

# Developing multidisciplinary mechanistic models: challenges and approaches

Daniel Vedder<sup>1,2,3</sup>, Samuel M. Fischer<sup>4</sup>, Kerstin Wiegand<sup>5,6</sup>, Guy Pe'er<sup>1,3</sup>

19th March 2024

<sup>1</sup> Department of Biodiversity and People, Helmholtz Center for Environmental Research - UFZ, Leipzig

<sup>2</sup> Institute of Biodiversity, Friedrich Schiller University Jena

<sup>3</sup> German Center for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig

<sup>4</sup> Department of Ecological Modelling, Helmholtz Center for Environmental Research - UFZ, Leipzig

<sup>5</sup> Department of Ecosystem Modelling, University of Göttingen, Germany

<sup>6</sup> Centre of Biodiversity and Sustainable Land Use (CBL), University of Göttingen, Germany

**Corresponding author:** Daniel Vedder, daniel.vedder@idiv.de

Puschstraße 4, 04103 Leipzig, Germany

1. Mechanistic models are a valuable tool for understanding and forecasting the dynamics of ecosystems in the face of global crises, such as biodiversity loss and climate change. However, current biodiversity models often struggle to adequately represent the complexity of the involved systems, as these are shaped by many different ecological, physical, and social processes. Consequently, we will need larger and more complex ecological models. Additionally, we will have to couple ecological models to models produced by other disciplines, such as climate science, economics, or sociology. Constructing such integrated models is a significant technical undertaking, which has received little attention by ecological modellers so far.
2. We review literature from computer science and several other environmental modelling disciplines to identify technical challenges with and approaches to creating large integrated models. We show that there is a software-architectural trade-off between modularity and integration, where the former is required to keep the technical complexity of a model manageable, and the latter is desirable to represent

the scientific complexity of a studied system. We then present and compare five different software engineering techniques for navigating this trade-off.

3. Which technique is most suitable for a given model depends on the model's aims and the available development resources. Simple models can be built monolithically, but larger models need to be subdivided into modules or packages to remain manageable. For very large or interdisciplinary models, model coupling on an ad-hoc basis or with a model coupling framework enables modellers to address problems spanning multiple domains or scales.
4. Other modelling disciplines have developed useful techniques for creating large integrated models. Ecological modellers need to learn from these disciplines and invest in increased software engineering expertise, if they want to build biodiversity models that are capable of jointly representing the numerous processes affecting ecosystems and biodiversity loss.

**Keywords: ecological modelling, mechanistic models, model complexity, model coupling, FAIR principles, research software**

## 1 Introduction

Mechanistic models (also known as process-based models) have established themselves as an important pillar of ecological research (Pilowsky et al., 2022). They help us better understand ecological processes and patterns (DeAngelis & Grimm, 2014), and are increasingly widely used to study the causes and effects of biodiversity loss (IPBES, 2016). In this, they show great potential for making ecology a more predictive science (McIntire et al., 2022; Stillman et al., 2016), as well as for supporting decision making (Grimm, Johnston et al., 2020; Will et al., 2021).

Mechanistic models are already used to model the full spectrum of biological scales, from individual-level genetic (Romero-Mujalli et al., 2019) and physiological processes (Sibly et al., 2013) all the way up to macroevolutionary processes that shape global patterns (Cabral et al., 2017). However, most ecological models only consider a very small number of processes (Urban et al., 2016), partly because of the complexity of ecosystems and the multitude of processes that need to be modelled. This is problematic, as gaining a full understanding of the natural world will require models that integrate multiple processes and organisational levels, including their interactions across scales (Grimm et al., 2017; Urban et al., 2022).

In addition to integrating the various strands of ecological research, mechanistic models

61 can be used to link ecology to other scientific disciplines. This is vital in the context  
62 of complex issues such as Global Change, where we need to understand how ecosystems  
63 and biodiversity affect and are affected by both physical domains such as climate (Urban  
64 et al., 2016) and socio-economic domains such as agriculture (Malawska et al., 2014).  
65 Ultimately, if we want to gain a deep, holistic understanding of the natural world we  
66 live in, we will not just need more comprehensive ecological models, but also integrated  
67 models that create a link between ecology and the physical and social sciences (Cabral  
68 et al., 2023).

69 Building such larger and more integrated models entails high scientific complexity, and  
70 there is a lively discussion among ecological modellers about whether and when this is  
71 necessary and how to deal with this (e.g. Lorscheid & Meyer, 2016; Sun et al., 2016; Top-  
72 ping et al., 2015). However, there is comparatively little discussion about the technical  
73 aspects of constructing large models. Models are software systems that also have a high  
74 technical complexity; thus, creating large integrated models will mean building large  
75 complicated software (Johanson & Hasselbring, 2018; Sanders & Kelly, 2008; Vedder,  
76 Ankenbrand & Cabral, 2021).

77 Of course, there are multiple dimensions in which model software can be improved, includ-  
78 ing increased realism and computational efficiency. However, with the growing impor-  
79 tance of interdisciplinary, and especially social-ecological, research, the aim of combining  
80 models from multiple domains has taken on new urgency (Vedder et al., submitted).  
81 While we should continue to think about how to build better monodisciplinary models  
82 (“go deep”), we should at the same time strive to build more multidisciplinary models  
83 (“go wide”).

84 Therefore, with this review, we address the question of how such model integration can be  
85 practically achieved. We juxtapose relevant principles from the computer science litera-  
86 ture on software engineering with examples from current practice in ecological modelling.  
87 To help link the two, we also draw on the wider literature on scientific computing, and  
88 include examples from other modelling fields such as climate modelling. We identify the  
89 challenges in creating large integrated models, and discuss the advantages and disadvan-  
90 tages of different techniques that can be used to build them. We end by drawing together  
91 concrete and practical advice for creating large integrated models.

### Box 1: Glossary of software terms

**Clean code** Computer code that is easy to read, understand, and modify (see Martin, 2009, for an in-depth discussion).

**Code base** The complete set of source code files for a software application, often taken to include the associated input files and documentation.

**Complexity ceiling** The maximum attainable complexity of a  $\rightarrow$ code base. As the size and technical complexity of a code base increases, the difficulty and cost of adding new features and fixing bugs increases further and further, partly due to accumulating  $\rightarrow$ technical debt. Eventually, further development becomes unfeasible and the software must be rewritten or left as-is. Good  $\rightarrow$ software engineering and  $\rightarrow$ clean code can raise the complexity ceiling (cf. Martin, 2009).

**Model coupling** The joining of two or more models, so that the output of one is used as input for another. May be accomplished using data files, software packages, network connections, or coupling frameworks (see sections 3.3 to 3.5, and the overview in Belete et al., 2017).

**Modularity** When referring to the internal structure of a  $\rightarrow$ code base: the property of being subdivided into semi-independent modules, or the degree of subdivision. Structuring software into self-contained modules makes it easier to understand and modify, as most changes will only affect a small subset of the entire code. (See Abelson et al., 1996, and McConnell, 2004, for detailed discussions.)

**Software architecture** The internal structure of a  $\rightarrow$ code base, including its organisation into packages, files, classes, and/or functions. Designing this is an important part of  $\rightarrow$ software engineering.

**Software engineering** The science and practice of developing software applications. The term emphasises the planning, design, and quality control procedures required for implementing large software projects (cf. McConnell, 2004). This is in contrast to the terms “programming” or “software development”, which often focus more on the actual act of writing code.

**Technical debt** Unnecessary technical complexity in a  $\rightarrow$ code base that makes it difficult to understand and work with. This may be caused by a  $\rightarrow$ software architecture that is either too simple or too complicated, a disregard of the principles of  $\rightarrow$ clean code, or incomplete documentation. Although writing such suboptimal code may be faster at first, the resulting (unnecessarily high) technical complexity makes future development harder and slower unless the software quality is improved (i.e. the debt is “paid back”).

## 2 The trade-off between modularity and integration

Large, interdisciplinary models are challenging to build both scientifically and technically (Vedder, Ankenbrand & Cabral, 2021). The larger model software becomes, the more its creation must be treated as software engineering and not merely as software development (Johanson & Hasselbring, 2018). Engineering large software systems is hard, and computer scientists have been thinking for decades about how to deal with their inherent and unavoidable complexity (see e.g. the seminal papers by Brooks, 1986; Dijkstra, 1972).

A fundamental solution to address this complexity is the concept of modularity, and the related concepts of encapsulation and abstraction (e.g. Abelson et al., 1996; McConnell, 2004). Complex software systems are easier to develop and understand when they are split into semi-independent subsystems. Two complementary aspects of modularity are “low coupling” and “information hiding” (Beck & Diehl, 2011). Low coupling means that each subsystem should be as self-contained as possible, with few links to the rest of the program. This makes it easier to develop, test, and analyse each subsystem in isolation. Information hiding means that each subsystem should have a defined and restricted interface through which the rest of the program can access its functionality without having to know the implementation details. This makes it possible to treat each subsystem as a “black box”, reducing the complexity of the complete system and making it much easier to think about and design. Additionally, it means that subsystems are easier to replace if and when that is necessary. Thus, the concept of modularity is directly applicable to the development of mechanistic models in ecology, and is indeed used in a similar manner to deal with scientific complexity (Lorscheid & Meyer, 2016).

However, the technical aim of keeping subsystems independent can come into conflict with the scientific desire to represent the numerous interlinkages between domains in the real world (Lippe et al., 2019; Topping et al., 2015). Many ecological models include interactions between processes at different scales (e.g. climate change and animal breeding behaviour), or between different entities at the same scale (e.g. predator and prey species). This requires the model source code to be sufficiently integrated to allow these interactions to be represented. On a technical level, the degree of integration of a software can be measured as the number of linkages between its components (e.g. the number of functions or variables in one component that are referenced outside of this component). The greater the number of linkages, the higher the integration and the lower the modularity (Beck & Diehl, 2011).

Therefore, there is a scientific desire for greater integration to increase realism and a technical desire for greater modularity to increase code tractability, leading to a trade-off

127 between these two model software properties. Modellers must be aware of this trade-off,  
128 and carefully weigh the scientific benefits of increased integration against its associated  
129 technical complexity costs. We therefore recommend the principle of writing model code  
130 that is “as modular as possible, as integrated as necessary”.

### 131 **3 Techniques for creating integrated models**

132 Below, we examine practical approaches for reconciling the scientific need for model  
133 integration with the technical imperative of software modularity. For this discussion, we  
134 use the terms “model” and “component” in a very specific sense. By “model” we mean a  
135 stand-alone executable software that is designed to represent one or more aspects of the  
136 physical world. By “component” we mean a subsystem of such a model, that handles one  
137 aspect of the model’s purpose and interacts with the model’s other components. Such  
138 a component may be a software module, package, or library, or even another model.  
139 Consequently, a stand-alone model may also be used as a component when it is coupled  
140 together with other components to create an integrated model. The definitions of model  
141 and component in this context are therefore functional and not mutually exclusive: a  
142 model is executable, a component interoperable.

143 Multiple techniques can be used to create large integrated models, each with their own  
144 benefits and drawbacks (Brandmeyer & Karimi, 2000). Fundamentally, the important  
145 questions are how to implement and link components. As complex software usually  
146 involves work by multiple developers or even teams of developers, the tasks of creating  
147 (and extending or adapting) components and models will often be done by different  
148 people and sometimes by different groups. It is therefore important to consider both the  
149 perspectives of component developers and model developers.

150 In this section we will present five techniques, which represent increasingly advanced  
151 types of software architectures that allow progressively greater levels of complexity to be  
152 handled (Fig. 1a). The techniques are characterised by differing degrees of interdepen-  
153 dence between the model and its components (Fig. 1b). Our selection of techniques is not  
154 meant to be comprehensive, but rather aims (1) to show the breadth of available options,  
155 (2) give examples of how they have been used in ecological modelling, and (3) discuss  
156 important differences between them. We do not propose that any of these techniques are  
157 always better or worse than the others; instead, we examine how well they suit specific  
158 research questions or organisational contexts. In this analysis, we focus on the seven  
159 aspects listed and summarised in Fig. 2.

### 3.1 Monolithic models

The simplest way to implement a mechanistic model is as a monolithic, purpose-built software that encompasses exactly those entities and processes relevant to the study question (Grimm & Railsback, 2005). Focusing on a specific question allows the developers to reduce complexity by excluding anything that is not directly necessary. At the same time, every part of the model can easily interact with every other part, allowing full integration. Hence, there is a low engineering overhead to the initial model construction. It is likely that the great majority of ecological models fall into this category, as modellers typically create new models for their specific needs and rarely share code (Bell et al., 2015; Berger et al., 2024).

The problem with this design is that, because every part of the code can influence every other part, the complexity of the code can end up increasing exponentially as new features are added. Eventually, the project may experience a “complexity ceiling” effect, where the code base has become so complicated that the developers struggle to expand it further without breaking existing functionality (Martin, 2009). This is why computer science developed modular programming techniques such as object-oriented programming, as these subdivide and thereby greatly reduce the complexity of code bases (cf. Brooks, 1986). Experience thus shows that the total complexity that can be represented with monolithic designs is much lower than with a modular design, and continuously adapting such models to new questions becomes harder and harder (Johanson & Hasselbring, 2018).

One example of an ecological model that was built with this technique is the GeMM model, which was designed to study eco-evolutionary dynamics of plant communities on islands (Leidinger et al., 2021). The original model design was well-suited to a number of questions relating to this study system (e.g. mechanisms of species invasions; Vedder, Leidinger and Sarmento Cabral, 2021). However, adapting the model to study terrestrial bird populations proved challenging and required the adaptation of large portions of code, making the whole code harder to understand (Vedder et al., 2022). Other examples of open-source models using the monolithic approach are the dispersal model of Sieger and Hovestadt (2021), the grazing models by Fust and Schlecht (2018) and Simon and Fortin (2020), or the butterfly model by Evans et al. (2019).

**Degree of integration:** Monolithic models offer maximal integration: every part of the code can access every other part.

**Contributors:** Monolithic models are typically built by individuals or small teams, who have a complete overview of the source code.

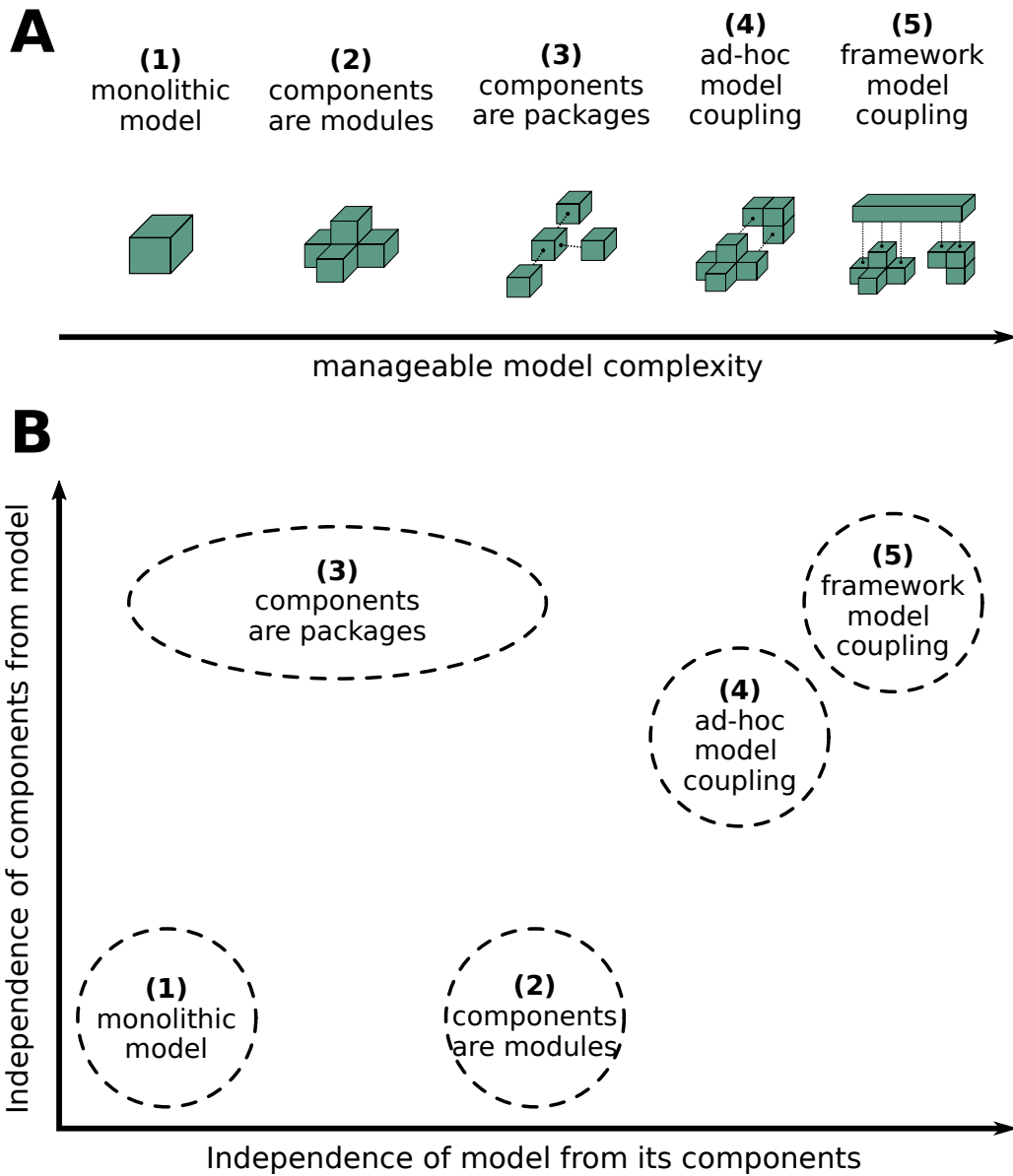


Figure 1: Different technical approaches to creating integrated models. The graph illustrates conceptually how independent components are of models and vice versa in each technique, i.e. how closely a specific component is tied to a specific model.



195 **Can combine languages:** Generally, monolithic models are built in a single program-  
196 ming language.

197 **Components are model-independent:** As monolithic models only have a single compo-  
198 nent, this component *is* the model and the two are not independent of each other  
199 in any way.

200 **Difficulty of creating components:** Creating a monolithic model is comparatively easy,  
201 as the software architecture is usually very simple and the overhead associated with  
202 packages or coupling frameworks is avoided. Also, although all parts have to be  
203 built by the developers, they have complete control over every aspect of their code.

204 **Difficulty of coupling components:** As monolithic models only have a single compo-  
205 nent, this question is not applicable.

206 **Difficulty of extending model:** Extending a monolithic model becomes progressively harder,  
207 as the lack of a clear internal structure leads to a rapidly mounting technical com-  
208 plexity that eventually precludes further development (“complexity ceiling”, see  
209 glossary in Box 1).

## 210 3.2 Components are modules

211 Modellers that anticipate having to deal with large numbers of entities and processes  
212 may adopt a more modular approach (Bell et al., 2015). This is also important if the  
213 model is expected to grow beyond the scope of the original study. The simplest way of  
214 increasing modularity is by internally subdividing the code base and clearly specifying  
215 how the different modules interact with each other. This will generally include splitting  
216 up the code into multiple files and folders, and can be aided by programming language  
217 features such as Python or Julia modules or C/C++ header files, as well as by classes  
218 and interfaces in object-oriented programming languages such as Java.

219 This subdivision requires a little forethought, and developers must be careful to keep  
220 the interaction between modules as limited as possible (McConnell, 2004). Still, such an  
221 architecture is not hard to set up, and offers large flexibility for integration where that  
222 is necessary. Thus, this technique is well-suited to models that include multiple domains  
223 with multiple interactions. It probably works best for small to medium-sized models and  
224 developer teams, as the still comparatively high degree of integration likely will pose a  
225 significant complexity burden for very large models that are worked on by many different  
226 people or multiple teams.

227 One example of a model that applies this technique to good effect is ALMaSS, which  
228 simulates animal species in agricultural landscapes (Topping et al., 2003). It includes

modules for multiple animal and crop species, a number that has been steadily growing over the last years (e.g. six animal species in Topping, 2011; seventeen in the 2022 code base, Topping, 2022). As another example, the macro-evolutionary model gen3sis uses a modular approach to allow the user to switch between different implementations of the simulated ecological and evolutionary processes (Hagen et al., 2021).

**Degree of integration:** Depending on the choice of programming language and modularisation technique (different files, classes, etc.), every part of the code can still access every other part where necessary. However, to keep up modularity, the developers should self-impose limits on the amount of integration they use depending on how much they consider necessary. This means that such models can have very different degrees of integration, but will generally be at a medium integration level.

**Contributors:** Modular models are typically built by small teams. Different team members will usually work on different sections, although all team members will have access to the complete source code.

**Can combine languages:** Generally, modular models are built in a single programming language.

**Components are model-independent:** Components in modular models are written specifically for the model they are a part of, and are therefore typically dependent on other parts of this particular model. Vice versa, the model does not have to be dependent on all of its components, with research questions often focussing on how enabling or disabling specific components (e.g. for land use dynamics) affects the overall model results.






























**Difficulty of creating components:** Each component is intended to be small and self-contained, making the creation of components easy.

**Difficulty of coupling components:** Because the developers have full control over all parts of the source code, aligning components with each other is straightforward.

**Difficulty of extending model:** The greater degree of modularity makes adding new functionality or even new components much easier than with monolithic models. However, because of the still relatively high degree of integration, these models are likely to hit their complexity ceiling earlier than models with a stronger separation between components (see the following techniques).

### 3.3 Components are packages

All major programming languages support packages, also known as libraries. This is software that is designed to be included in other programs in order to perform a specific

	(1) monolithic model	(2) components are modules	(3) components are packages	(4) ad-hoc model coupling	(5) framework model coupling
structure					
degree of integration					
contributors					
can combine languages	✗	✗	(✓)	✓	(✓)
components are model-independent	✗	✗	✓	(✓)	✓
difficulty of creating components					
difficulty of coupling components	n/a				
difficulty of extending model					










 low integration	 single team	✓ yes	 easy
 medium integration	 collaborating teams	(✓) sometimes	 medium difficulty
 high integration	 research community	✗ no	 hard

Figure 2: Different software engineering techniques have different advantages and drawbacks, making them suitable for different modelling purposes and contexts. This figure offers a qualitative comparison of a number of relevant points as a summary.

task, such as statistical analysis or visualisation. Packages are generally not built to be used as stand-alone executables. They are nonetheless independent of the programs they are embedded in, and are usable by any program with similar requirements. Thus, whereas modules (in the sense discussed above) are components that are created for and used solely within a specific model, packages are components that are meant to be used by many models. This is achieved by defining an API (application programmer interface) to specify the functions and classes that the given package provides, which input data it requires, and what output it produces. Because packages are largely self-contained, they provide a greater degree of modularity than modules. This becomes important as models grow in size, particularly if the model components are created by multiple developer teams.

By adhering to the specifications for creating packages in their chosen programming language, component developers can make their code interoperable and easily accessible to other model developers. Many programming languages offer package repositories to enable rapid dissemination of software, such as CRAN for R (cf. Ram et al., 2019), pip for Python (cf. Maji et al., 2020), and Pkg.jl for Julia (cf. Churavy et al., 2022). Using preexisting packages as model components allows model developers to greatly reduce the amount of work they have to do themselves, while automatically making the code more modular and thus more understandable. In some cases (particularly with compiled packages known as dynamically-linked libraries), it can also be possible to include code written in a different programming language in a model, thus allowing developers to benefit from a wider circle of previous work. On the downside, a package may not offer all the features the model developers would like, require the model code to be adjusted to fit the package requirements, or induce coding overhead for packaging and maintenance. Although many ecologists are familiar with the concept of packages for data analysis (cf. Marwick et al., 2018), using packages as model components is not as widely spread. One example is the plant growth model by Schouten et al. (2020), who split up their model code into three independent packages that can also be used for other models. It is also an option to transform complete ecological models into packages, thus making them components that can be used by others. For example, this was done for the Madingley (Harfoot, Newbold et al., 2014; Hoeks et al., 2021) and RangeShifter models (Bocedi et al., 2021; Malchow et al., 2021) in order to make them interoperable with R.

**Degree of integration:** Packages are designed to offer a public interface, a set of functions and/or classes that can be called by users of the package, while making their internal workings inaccessible to users. This makes for strong modularity, but consequently low integration.

299 **Contributors:** Often, every package in a software project is developed by a separate  
300 team. Teams may or may not collaborate explicitly, e.g. by adjusting a package to  
301 provide functionality required for a specific application.

302 **Can combine languages:** Many programming languages can be combined with packages  
303 built in other languages, although this may be difficult to set up.

304 **Components are model-independent:** Packages are usually built to provide general func-  
305 tionality independent of a specific use case, and hence independent of the model  
306 they are included in. How dependent a model is on a given package depends on  
307 the availability of other packages offering equivalent functionality.

308 **Difficulty of creating components:** Every programming language has its own guidelines  
309 on how to create packages. Designing a good package API takes some thought, as  
310 it must consider both the current and future needs of package users as well as those  
311 of the developers.

312 **Difficulty of coupling components:** Loading packages into a software is designed to be  
313 simple, and packages often offer good documentation of their functionality. The  
314 largest difficulty comes from the model developers not having complete control over  
315 the source code of the package, so that they may have to adapt their model to the  
316 utilised packages.

317 **Difficulty of extending model:** Due to the high modularity of a package-based design,  
318 adding new functionality later on is not more difficult than the original model  
319 creation.

### 320 3.4 Ad-hoc model coupling

321 Sometimes, developers want to link two or more full models together to explore inter-  
322 domain effects and feedbacks. This is known as model coupling, and can be achieved by  
323 multiple technical means (Belete et al., 2017; Robinson et al., 2018). The simplest way  
324 is to adapt one or more of the models so that they can use each others' output files as  
325 input, and then run them sequentially if no feedbacks exist, or update them step-by-  
326 step in turn if feedbacks do exist. Instead of using files (which is simple, but likely to  
327 be very slow), the data exchange can also be implemented using a network connection,  
328 or by loading the components as packages (see above). In any case, the result is an  
329 integrated model whose components are themselves stand-alone models, but that have  
330 been adapted to specifically interact with each other. As this adaptation must be done  
331 for each set of models on a case-by-case basis, we refer to this form of coupling as “ad-hoc

332 model coupling”, to differentiate it from the more generic “framework model coupling”  
333 (see below).

334 Ad-hoc model coupling is well-suited for collaborations among a small number of devel-  
335 opment teams. Because the undertaken adaptation is specific to the target models, a  
336 relatively high degree of integration can be achieved. It is also often possible to couple  
337 models written in different programming languages. However, having to adapt two or  
338 more existing models to each other is finicky work that becomes rapidly more complex  
339 the more models are involved. Therefore, although this technique can be useful for cou-  
340 pling two or three models, it is not feasible for building large collections of interoperable  
341 models.

342 Ad-hoc model coupling was used, for example, by Synes et al. (2019) to combine the eco-  
343 logical movement model RangeShifter with the socio-economic land-use model CRAFTY.  
344 This allowed the authors to study the feedbacks between land use, crop yield, and polli-  
345 nator abundance. Robinson et al. (2018) describe several other examples of ad-hoc model  
346 coupling, including a three-model coupling of the dynamic global vegetation model LPJ-  
347 GUESS with the climate model IMOGEN and the food system model PLUMv2. These  
348 were used to study interlinkages between agricultural intensification and expansion and  
349 climate change.

350 **Degree of integration:** While each component model is originally self-contained, the in-  
351 dividualised coupling process allows developers to connect components quite closely  
352 to each other, thus achieving an intermediate degree of integration.

353 **Contributors:** Ad-hoc model coupling is generally used to bring together the work by a  
354 small number of developer teams.

355 **Can combine languages:** As ad-hoc coupling usually does not require source code com-  
356 patibility (e.g. when coupling via input/output file exchange), models written in  
357 different programming languages can be combined as they are.

358 **Components are model-independent:** Because each component is itself a model, com-  
359 ponents are technically independent of each other. However, the coupling process  
360 may involve adapting the constituent models to be able to interact with each other,  
361 so there is a greater degree of mutual dependence than with framework coupling.

362 **Difficulty of creating components:** The difficulty of creating each component model de-  
363 pends strongly on its own complexity. Planning for model coupling already during  
364 the design phase of a model allows the component model to be kept minimal and  
365 at a lower level of complexity, thus reducing the difficulty of implementation.

366 **Difficulty of coupling components:** Coupling models on an ad-hoc basis can be tricky,

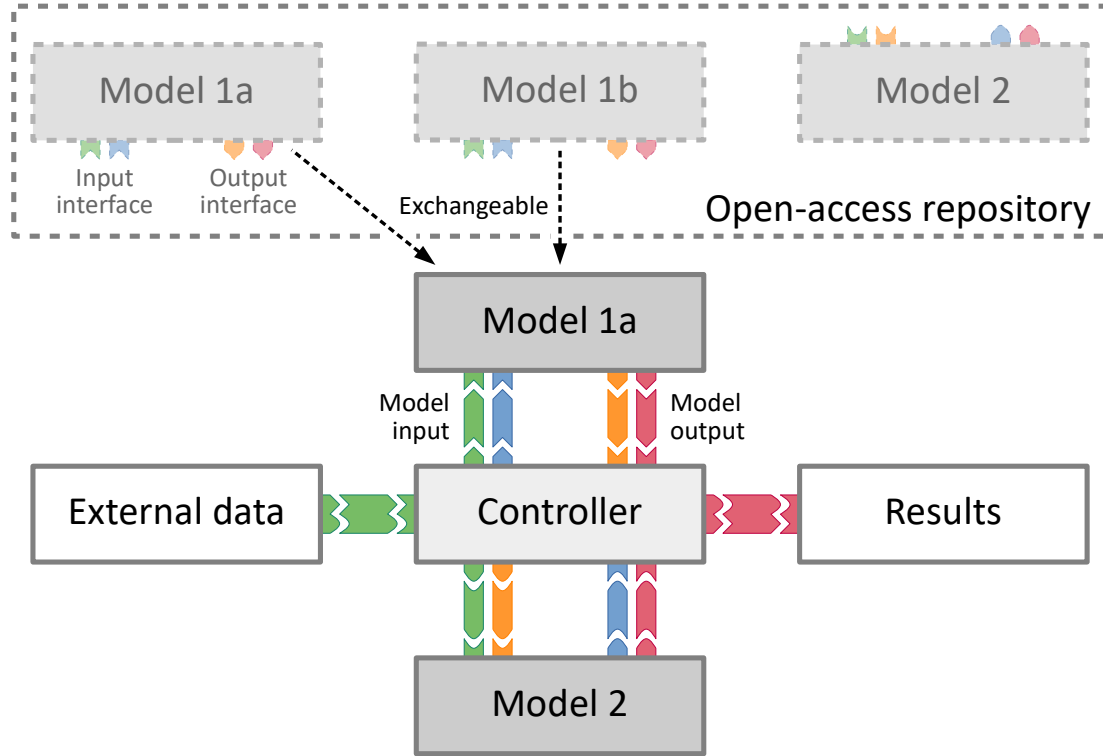


Figure 3: Conceptual depiction of a model coupling framework. Individual models are available from an open-access repository, and declare their required input and output variables using the standardised interface defined by the coupling framework. Modellers select relevant models from the repository (or build their own), and link them using a controller software provided by the coupling framework, which manages scheduling and data exchange.

367 as input and output data have to be carefully aligned. Modellers not only have to  
 368 ensure that the component models are scientifically compatible (e.g. by convert-  
 369 ing between units or different representations of space), but also need to set up  
 370 the technical communication between components (e.g. through file exchange or  
 371 network connections).

372 **Difficulty of extending model:** Because the components are specifically aligned to each  
 373 other, extending an ad-hoc coupled model further involves a lot of detail work to  
 374 integrate new components with the existing structure. This may rapidly become  
 375 unfeasible.

## **Box 2: Case study I: integrated models in climate/earth-system models**

Climate models have been pushing the boundaries of what is computationally and scientifically possible since the 1950s (Edwards, 2011). Initially, these models were restricted to atmospheric processes, but soon began to be linked to other earth-system models, such as for the oceans or the cryosphere. In 2003, the Earth System Modelling Framework (ESMF) was introduced in order to encourage and facilitate this growing cooperation between institutes and disciplines (Hill et al., 2004). The ESMF consortium created a framework that could be used to integrate existing models into a single application. It worked by defining a “superstructure” (a basic software interface that component models could connect to) and providing an “infrastructure” (a collection of utility functions to help components communicate with each other). On the basis of this, the Earth System Prediction Suite (ESPS) was later set up to provide a curated collection of models that conform to the relevant standards and can therefore be expected to be readily interoperable (Theurich et al., 2016).

Importantly, the parallel development of multiple, competing modelling approaches fostered positive competitiveness and robustness in climate science, by exploring the range of possible future climate scenarios according to different models (J.-Y. Lee et al., 2021). This community approach to modelling has been formalised in the Coupled Model Intercomparison Project (CMIP; Eyring et al., 2016). The consistency with which greenhouse gas emissions were shown to drive climate change has given these modelling results a very high level of confidence with respect to the anthropogenic contribution to climate change. Thus, as simple as the question may be (e.g. “What is the effect of anthropogenic greenhouse gases?”), delivering a robust reply was very much achieved by integrating models, including complex interactions, and testing multiple models (Manabe, 2019). Moreover, only through such integration could tipping points be studied and further explored (Armstrong McKay et al., 2022).

This MIP approach (comparing the output of multiple models using standardised input data), pioneered by climate modelling, has since been extended to other modelling discipline. Examples include the Inter-Sectoral Impact Model Intercomparison Project (ISI-MIP, Rosenzweig et al., 2017), which also considers ecosystems, or the Biodiversity and Ecosystem Services Scenario-based Intercomparison of Models (BES-SIM, Kim et al., 2018).



### 376 3.5 Framework model coupling

377 The climate and earth science modelling communities were the first to realise the need  
378 for easy interoperability of diverse models, and pioneered the technique of framework  
379 model coupling (Box 1). A coupling framework defines a standard interface that all  
380 compatible models have to conform to, thus removing the need for case-by-case model  
381 adaptations. It also provides a central software to coordinate the execution of the coupled  
382 models (the controller), as well as utility functions to help with unit conversions, spatial  
383 and temporal scale alignment, and other practicalities of model coupling (Belete et al.,  
384 2017). This means that although model developers have to do some work to adapt their  
385 model to a given coupling framework, the model is then (at least in theory) compatible  
386 with any other model adapted to the same framework (Fig. 3). Achieving this kind of  
387 standardisation requires a very high level of coordination among researchers, but has  
388 proven highly valuable not just in climate and earth system modelling, but also in other  
389 modelling fields like agriculture (Box 2).

390 Multiple coupling frameworks are available, often originating in different modelling dis-  
391 ciplines and differing in their specificity and ease of use (Knapen et al., 2013). The most  
392 general framework at the moment is probably OpenMI (Gregersen et al., 2007; Harpham  
393 et al., 2019), which was first developed by hydrological modellers but is now also used  
394 to link models in other fields, such as agriculture (S. Janssen et al., 2011), economics  
395 (Bulatewicz et al., 2010), or pathogen ecology (Shrestha et al., 2013). So far, however,  
396 coupling models using frameworks is still very rare in ecology, despite the technique’s  
397 proven potential for achieving large-scale model integration as called for by Urban et al.  
398 (2022) and others.

399 **Degree of integration:** Adapting models to be used as components in framework cou-  
400 pling requires giving them a standardised API (similar to packages). Therefore,  
401 the interaction possibilities with each component are clearly defined and restricted,  
402 resulting in a strongly modular architecture with a medium to low degree of inte-  
403 gration.

404 **Contributors:** The up-front cost of adapting a model to a framework is only worth-  
405 while if many other models also use this framework. Therefore, establishing a  
406 coupling framework requires a high amount of coordination among many different  
407 teams of modellers. Once this barrier has been surmounted, the advantage is that  
408 any framework-compatible models can be easily linked, thus enabling collaboration  
409 across a wide range of teams and disciplines.

410 **Can combine languages:** Most frameworks support a specific set of programming lan-

411 guages. Models that want to use a framework therefore must either be written in  
412 one of these languages, or provide a wrapper for one of them (e.g. through an R or  
413 Python package).

414 **Components are model-independent:** In framework coupling, each component is a sep-  
415 arate model that can also be used on its own, or in combination with other models  
416 in a different integrated model. Thus, there is maximum independence of the com-  
417 ponents from the model.

418 **Difficulty of creating components:** As each component is itself a model, the difficulty  
419 of creating it depends on its own type and complexity.

420 **Difficulty of coupling components:** Adjusting a component model to be compatible  
421 with a framework can be a bit of work, but once this has been done, coupling  
422 models within the framework is designed to be quick and easy.

423 **Difficulty of extending model:** Extending an integrated model is very simple, as long  
424 as any new components are compatible with the coupling framework.

## 425 4 Practical recommendations

426 Moving on from the overview of techniques, in this section we offer recommendations on  
427 how to use these techniques in practice. We are guided by three questions: (1) Which  
428 technique is best suited for my purposes? (2) How can I build components that are  
429 readily interoperable with components and models developed by others? (3) How can I  
430 build models that integrate existing components? We summarise our recommendations  
431 in table 1.

### 432 4.1 Choosing a technique

433 The first question to ask when selecting a technique at the beginning of a new mod-  
434 elling project is: How large and complex should the model become? The greater the  
435 desired complexity, the more important it is to use a more advanced technique (Fig. 1a;  
436 Johanson and Hasselbring, 2018). On the other hand, a more advanced technique may  
437 be unnecessarily complicated to use for a simple model. If a model is only intended to  
438 be used for a single, well-defined study, a monolithic model is likely to be the simplest  
439 and most efficient option (Section 3.1). If it should be used for multiple studies, and  
440 potentially further extended in future, a modular architecture is highly advisable. If all  
441 parts of the model can or should be written by the team itself, this would mean using

### **Box 3: Case study II: integrated models in agricultural sciences**

Agriculture is another research field that has a long history of modelling. Several traditions of agricultural modelling may be identified. First, crop-growth models are used to predict yields under varying management regimes and environmental conditions (Pan & Chen, 2021). Secondly, farm models are used to assess (primarily economic) policy impacts both on individual farms and on the regional agricultural sector (Reidsma et al., 2018). Agricultural processes or systems are also included in models from fields such as human geography, environmental sciences, and ecology (e.g. Le et al., 2008; Schmidt et al., 2017; Topping et al., 2003).

Although coming from different disciplinary backgrounds, different model types are increasingly being combined in order to address questions that require multiple perspectives. For example, Piorr et al. (2009) coupled economic and environmental models to assess the likely effects of the European Common Agricultural Policy on production and ecosystem health, while Malawska and Topping (2018) did so to investigate the effects of market shifts on farmland species. More comprehensively, Schreinemachers and Berger (2011) created an integrated model with components for farm economics and technology, crop growth, water flow, and soil erosion and nutrients.

The merging of modelling disciplines is being encouraged by large-scale projects such as the EU's SEAMLESS, which aims to integrate socio-economic and environmental models across scales for policy assessments (S. Janssen et al., 2011; van Ittersum et al., 2008), or the Agricultural Model Intercomparison and Improvement Project (AgMIP), which seeks to bring together crop-growth, farm, and climate models (Rosenzweig et al., 2013). To help this exchange among modellers, the US Department of Agriculture pushed development of the Object Modelling System (OMS), a lightweight environmental modelling framework similar to the ESMF (David et al., 2013), while the Agricultural Model Exchange Initiative (AMEI) aims to establish a modelling community similar to the ESPS (Enders et al., 2018). Although the use of scientific models in agricultural policy-making is still limited, these efforts are establishing a base of knowledge that is increasingly being drawn on for policy impact assessments by governments and international organisations and agreements, for instance in the European Union (Reidsma et al., 2018).

Table 1: Practical recommendations for creating large, integrated models, or components for such models. See section 4 for details.

<b>Aim</b>	<b>Recommendations</b>
choosing a technique	<ul style="list-style-type: none"> <li>▪ identify how complex the model should be</li> <li>▪ identify whether suitable components are already available</li> <li>▪ examine what software expertise is / is not available in the team of collaborators</li> <li>▪ envision how the model should or could be used in future</li> </ul>
building interoperable components	<ul style="list-style-type: none"> <li>▪ follow good coding practice</li> <li>▪ provide detailed documentation</li> <li>▪ make source code public</li> <li>▪ provide software as a package</li> <li>▪ provide bindings to coupling frameworks</li> </ul>
building integrated models	<ul style="list-style-type: none"> <li>▪ choose modular software architectures</li> <li>▪ build on existing software where possible</li> <li>▪ collaborate with other modellers</li> <li>▪ learn from other modelling disciplines</li> <li>▪ utilise coupling frameworks</li> </ul>

“components as modules” (Section 3.2); if existing libraries or packages can be used it becomes “components as packages” (Section 3.3). For larger models that integrate across domains, coupling with existing models can be helpful or even essential, either with ad-hoc coupling (Section 3.4) or with framework coupling (Section 3.5).

For any medium- or larger-sized model, the second question is therefore to find out whether there are suitable components or models already available that can be utilised (either as packages, or for model coupling). These can be searched for using e.g. Google Scholar, Github, or CoMSES (Rollins et al., 2014). To assess whether a component or model is suitable, the following questions can help: Does it include the processes and state variables that are relevant to my research question? Do I have the required input data available? Is the software open source, and is it well-documented? Does it have an active user community, and/or are the developers easy to contact? When deciding whether or not to use externally developed software components, one must weigh the cost of working with software that may not be a perfect match for the project requirements against the cost of having to develop the desired functionality internally (“buy vs. build”, cf. Brooks, 1986).

The third question is the available expertise and experience in software development

among the team members. While monolithic models (Section 3.1) can be constructed by anyone who knows how to program, the other techniques require a little more knowledge of software engineering principles and tools. In particular framework model coupling (Section 3.5) has quite a steep learning curve. If the study question requires one of the more advanced techniques, researchers may decide to invest the time to learn the necessary skills themselves, collaborate with other researchers who have the expertise, or employ professional developers (Cohen et al., 2021).

Finally, it is good to have at least a vague idea of how the model to be built could or should be used in future. The longer it is to be used and the more people are to use it, the more important it is to use one or several of the more advanced techniques (cf. the experiences with the FORMIND model, Box 4). Although these come with a greater up-front cost in designing the software architecture and setting up the code base, they make it significantly easier to extend the model in future and to use it together with software written by other researchers (Fig. 2).

## 4.2 Building interoperable components

An important insight is that the road to large complex models starts with the development of small interoperable ones. Therefore, if as a modelling community we want to work towards developing larger models, individual modellers need to become better at building components and models that can easily be linked up with others (Bell et al., 2015; Berger et al., 2024).

To build components that can be readily integrated into large models, the aim should be to create high-quality scientific software products that are as easy as possible for other researchers to (re-)use (McIntire et al., 2022; Sanders & Kelly, 2008). This requires rigorous application of the FAIR criteria: Findable, Accessible, Interoperable, and Reusable (Barton et al., 2022; Hasselbring et al., 2020). Essentially, this boils down to learning and following best practices for software development in computational science in general (Balaban et al., 2021; Wilson et al., 2014) and ecological modelling in particular (Ropella et al., 2002; Scheller et al., 2010; Vedder, Ankenbrand & Cabral, 2021).

Important principles here are writing clean code (Filazzola & Lortie, 2022), using version control for open-source development (Perez-Riverol et al., 2016), using automated testing and code reviews for verification (Holzworth et al., 2011; Vable et al., 2021), and providing good technical and scientific documentation (Grimm, Railsback et al., 2020; B. D. Lee, 2018). Communities such as rOpenSci can help modellers write better software by providing detailed technical reviews (Ram et al., 2019). Creating high-quality software

493 is important to make the code accessible and usable by others. It also makes code easier  
494 to extend by avoiding “technical debt”, i.e. unnecessary technical complexity that slows  
495 down future development (see Glossary).

496 It is crucial that ecological modellers make all their source code openly available and  
497 document it sufficiently, not only for the sake of scientific reproducibility but also to  
498 enable others to build on the components they created (M. A. Janssen et al., 2020). This  
499 can be done on general-purpose platforms like Github (for collaborative development) or  
500 Zenodo (for code archiving). More narrowly modelling-oriented platforms can provide  
501 additional benefits, by acting as central repositories that make finding useful models and  
502 components quick and easy (Bell et al., 2015). One such platform is CoMSES, a library  
503 of agent-based and individual-based models that is seeing widespread use in the social  
504 sciences but is still little known among ecologists (M. A. Janssen et al., 2008; Rollins  
505 et al., 2014).

506 Modellers should also form the habit of making their software available as installable  
507 packages in their preferred programming language, ideally in a standard package reposi-  
508 tory (e.g. PyPI for Python or CRAN for R). This lowers the bar for installing components  
509 considerably, making it easier for other researchers to build on existing work.

510 To improve dissemination of new research software, several journals now allow develop-  
511 ers to publish descriptions of applications and packages as a separate article type (e.g.  
512 *Methods in Ecology and Evolution*, *Journal of Open Source Software*). This has the addi-  
513 tional benefit of providing scientific incentive (i.e. publications) for releasing code, which  
514 is particularly valuable for early-career researchers.

515 As ecological models become larger and more complex, the importance of coupling frame-  
516 works will increase. This is particularly true as ecologists seek to couple their models  
517 to models from fields that already use such frameworks, including the physical and so-  
518 cial sciences. Therefore, ecologists should learn about existing frameworks and acquaint  
519 themselves with their use (Belete et al., 2017; Knapen et al., 2013). Seen from the per-  
520 spective of a component developer, making a component compatible with an established  
521 coupling framework would be a major step toward interdisciplinary model interoperabil-  
522 ity.

523 Finally, model interoperability would be greatly aided by the adoption of a unified set of  
524 Essential Biodiversity Variables as standardised input/output variables for models (Jetz  
525 et al., 2019). This would enable harmonisation of model results and ease model coupling,  
526 as well as make it easier to interface models with empirical data sources (Fer et al., 2021;  
527 Urban et al., 2022). A coordinated move in this direction would be especially effective

528 if accompanied by a standardisation of metadata, such as for the recently proposed  
529 Reusable Building Blocks (Berger et al., 2024).

### 530 4.3 Building integrated models

531 As ecologists think about creating large, complex models integrating many different en-  
532 tities, processes, and domains (e.g. Urban et al., 2016; Urban et al., 2022), they need to  
533 think very carefully about the technical challenges this entails. Building large software  
534 well is a significant undertaking, especially as software complexity does not scale linearly  
535 with software size (McConnell, 2004). Research teams need to consider the resources that  
536 are available for development, including time, money, manpower, and know-how. Based  
537 on this, they must decide what level of scientific complexity can be feasibly modelled,  
538 and which integration technique is most suitable to their purpose and context (Section  
539 3, 4.1).

540 When attempting to build large models, researchers must realise the importance of care-  
541 fully planning the code’s design and architecture. For this, it is useful to have team  
542 members who have trained in software engineering (Cohen et al., 2021). Studying well-  
543 known open-source programs is also an excellent way to learn more about good software  
544 architecture and current practices in software development (e.g. Brown & Wilson, 2011).

545 The experience of other modelling fields shows that eventually, model complexity grows  
546 to such a degree that coupling frameworks are often the most effective way to further  
547 growth (Box 2,3). Ecological modelling does not seem to have reached this point yet, but  
548 considering the increasing amount of integration of ecological models with climate, hy-  
549 drological, economic, sociological and other models, it can be expected that the field will  
550 reach this stage soon. This is a promising development, but one that brings its own set  
551 of challenges. Model coupling not only involves adaptation of existing software, but also  
552 requires models to be made scientifically compatible with regards to spatial and tempo-  
553 ral scales and input and output data (Belete et al., 2017; Brandmeyer & Karimi, 2000).  
554 Coupling frameworks can greatly help with this process, but add their own complex-  
555 ity overhead. Complicating matters is the range of available coupling frameworks, each  
556 established in different disciplines and available for different programming languages.

557 It should be noted that it is not an aim that all ecological models should be large and  
558 integrated, or that all modellers need to work with framework model coupling. Smaller  
559 models have their place (Sun et al., 2016), and all techniques can be useful (Section 4.1).  
560 However, as argued above, in addition to the small and medium-sized models we already  
561 have, we will need larger and integrated models to study the interdisciplinary questions

562 now facing science.

563 In view of all this, it seems an important challenge for the next years of ecological  
564 modelling to become better at building these integrated models. This will include training  
565 modellers in software development, as well as establishing conventions and standards for  
566 model publication and coupling. While other fields have been successfully using coupled  
567 models for decades, such coupling is rarely done in ecological modelling. This is an area  
568 where the recently-formed Open Modelling Foundation could be a vital catalyst for future  
569 methodological developments (Barton et al., 2022).

## 570 **5 Discussion**

### 571 **5.1 The need for large integrated models**

572 Computational models have become essential instruments for scientific research and pol-  
573 icy advice. They play a central role in the work of both the IPCC (e.g. Eyring et al.,  
574 2016) and IPBES (e.g. IPBES, 2016), helping us better understand the global crises of  
575 climate change and biodiversity loss, and the interlinkages between them (Pörtner et al.,  
576 2021). However, the use and acceptance of models is much better established in climate  
577 change policy than in biodiversity policy (Urban et al., 2022). This is partly due to insuf-  
578 ficient and misaligned communication between modellers and decision-makers (IPBES,  
579 2016; Will et al., 2021), but also because biodiversity is often not well integrated into  
580 models of social-ecological systems (Vedder et al., submitted).

581 In the face of an ongoing ecological crisis, ecologists seek not only to understand Global  
582 Change processes but also to provide relevant and timely advice to policy makers and  
583 stakeholders. To do so, we will need increasingly advanced models that can provide  
584 insight into the multi-scale, multi-domain systems that we study. This requires expanding  
585 our models beyond their current focus on a small number of ecological processes, and  
586 embrace the complexity of real-world systems with their multi-scale pressures (Topping  
587 et al., 2015; Urban et al., 2022). This can only be effectively done by developing a  
588 practice of interdisciplinary modelling.

589 This is relevant in two directions. First, ecological modellers need to link their models to  
590 models of other physical systems. There is a strong tradition of mechanistic modelling in  
591 several disciplines in the environmental sciences, most notably in climate science, but also  
592 in areas like hydrology, ecotoxicology, and earth system science more generally. Ecologists  
593 can profit from and contribute to existing model coupling initiatives, such as OpenMI  
594 (Harpham et al., 2019), various Integrated Assessment Models (Harfoot, Tittensor et al.,



#### Box 4: Case study III: life history of a large ecological model

FORMIND (Bohn et al., 2014; Fischer et al., 2016; Köhler & Huth, 1998) is a process-based forest model incorporating regeneration, competition, growth, and mortality of trees. As individuals are modelled explicitly, the model allows a detailed analysis of forest structure and productivity under varying environmental conditions. FORMIND has a modular design, allowing the base model to be adjusted to a wide range of research questions, including the effects of forests fragmentation (Pütz et al., 2011), landslides (Dislich & Huth, 2012), water competition and droughts (Gutiérrez et al., 2014), and wild fires (Fischer, 2021).

The components are coupled via the “**components are modules**” strategy. Nonetheless, model and components remain strongly linked, to facilitate the exchange of data and the integration of components into the model’s main routines. This architecture made it easy to add new components to the model without major changes to the historic core. However, with a growing number of modules, the code base became progressively more complex, making it increasingly difficult to update the model without breaking functionality.

In recent years, FORMIND has been combined with external software via **ad-hoc coupling** methods, e.g. to fit the model to field data (Lehmann & Huth, 2015). Building on the model’s text file interface for data exchange reduced the need for code changes but also limited flexibility and created a significant computational overhead. Hence, a Python package wrapping the original C++ code is under development, allowing users to read and manipulate parameters and state variables at runtime (“**components are packages**”; first application in [Fischer et. al., manuscript in preparation]).

Currently, FORMIND is also being coupled with an external soil moisture model (Samaniego et al., 2010) to study forest-soil interactions. As the two models run at different temporal and spatial scales and efficient data exchange is required for the intended large-scale simulations, the Python-based framework FINAM (Lange et al., 2023) is used to couple the models (“**framework model coupling**”). Implementing the FINAM interface for FORMIND did not require changes to the existing model and only minimal additional code. As the FINAM interface is model-agnostic, the interface can also facilitate the integration of FORMIND into comprehensive landscape-scale models of the environment (cf. Cabral et al., 2023; Urban et al., 2022).

2014), or ISI-MIP (Rosenzweig et al., 2017).

Secondly, ecological modellers should become more involved in the burgeoning field of socio-ecological systems research. There have been significant recent advances in coupling ecological and socio-economic models (e.g. Guillem et al., 2015; Synes et al., 2019). Still, there are many challenges in incorporating mutual feedbacks between human and natural systems (Farahbakhsh et al., 2022), and in representing the multiple scales relevant to many socio-ecological systems (Lippe et al., 2019). Altogether, scaling up our understanding of socio-ecological systems, including telecoupled systems, cannot be achieved without much more complex models than currently exist.

Ultimately, addressing sustainability challenges requires models that combine all three domains: the ecological, the physical, and the human. For instance, when studying land use change, it is desirable to combine models from multiple fields, including human geography, ecology, and climate science, in order to understand how processes in each of the three domains influence processes in the other two (Cabral et al., 2023).

## 5.2 A way forward

To meet the scientific and technical challenges of creating large integrated models, ecological modellers should invest into software engineering training, as well as into intra- and interdisciplinary standardisation processes.

In this paper we have introduced a set of software engineering techniques for building models of different sizes and complexities. Which technique is best suited to a given research context depends on the aim of the model, the available development resources, and the likely future users of the model. The larger a model becomes, the more important it is to carefully plan its software architecture and to follow good software engineering practices (Johanson & Hasselbring, 2018). As a model grows over time, it is also likely that new techniques will become relevant, as exemplified by the forest model FORMIND (Box 3).

Like many other computational scientists, ecological modellers face the problem that few have had good training in software engineering (Nowogrodzki, 2019). Although this is understandable given the contents of most ecology curricula in universities (Farrell & Carey, 2018), it frequently results in code that ignores the most basic principles of software quality and validation (Prabhu et al., 2011). This issue not only undermines the credibility of our scientific models, but also impedes researchers' ability to utilize and expand upon existing software. (Sanders & Kelly, 2008). It is therefore imperative that we invest into better software training for modellers, and collaborate with professional

629 software developers to produce reliable and usable model code (Cohen et al., 2021).

630 We recognise that this currently faces a number of institutional barriers. Some relate to  
631 finances: smaller research groups often lack the funds to hire professional developers, and  
632 getting funding to develop and maintain research software can be difficult (Nowogrodzki,  
633 2019). Furthermore, research institutes often cannot offer the job security or salaries  
634 that are competitive with those of software developers in industry. Other barriers relate  
635 to culture: because research software is often not valued in itself, but only for the sci-  
636 entific output it produces, little importance is attached to tasks that make the software  
637 itself better, such as improving code quality and ensuring appropriate documentation  
638 (Johanson & Hasselbring, 2018). Especially early-career researchers in modelling may  
639 be pressured to “produce results” as fast as possible, leaving them little time to gain  
640 the technical skills needed to produce more complex software. This in turn contributes  
641 to the “yet another model” syndrome, i.e. the observed profusion of simple models at  
642 the expense of more advanced ones (O’Sullivan et al., 2016). We therefore propose that  
643 to create more complex models, ecological modellers should invest in becoming better  
644 software developers. This will require a cultural shift to value code as a scientific output  
645 in its own right (Mislán et al., 2016).

646 Beyond simply improving the quality of model software, ecological modellers also need  
647 to think more about standardisation of data and metadata, both within ecology and  
648 with other disciplines. Within ecology, increased use of online model repositories such as  
649 CoMSES would aid the discoverability of models and model components (Bell et al., 2015;  
650 Rollins et al., 2014). Further development and use of standardised Essential Biodiversity  
651 Variables could help to align the input and output variables of different models, and of  
652 models with empirical data sources, thus allowing easier coupling (Urban et al., 2022).  
653 Programs such as BES-SIM can help harmonise the results of ecological models, and  
654 contribute to a more unified and strategic development of the field (Kim et al., 2018). To  
655 collaborate with disciplines outside ecology, ecological modellers need to learn more about  
656 existing standards, frameworks, and collaboration networks. Here, the Open Modelling  
657 Foundation is a valuable initiative to bring together modellers from numerous domains  
658 to promote collaboration and standardisation (Barton et al., 2022). Not least, we can  
659 use such connections to learn about how other modelling disciplines have solved the  
660 challenges our field currently faces, as many of these disciplines are methodologically  
661 much further advanced than ecological modelling.

## 6 Conclusion

To advance ecological modelling, we will need to create larger and more integrated mechanistic models. This is particularly urgent in light of the growing demand for interdisciplinary modelling to face the dual crises of climate change and biodiversity loss. We must learn not only to build comprehensive models of biodiversity and ecosystems, but also to couple these with climate, land use, economic, and other models.

In this review, we highlight the inherent trade-off between integration and modularity, and explain the associated tension between scientific requirements and technical constraints. We showcase five different integration techniques and how they are currently being used, as well as discussing their relative strengths and weaknesses. As practical recommendations, we emphasise that ecological modellers need more training in software engineering, must adopt FAIR research practices, and should begin to think about how best to apply existing coupling techniques to ecological models.

## Acknowledgements

The authors wish to thank Quillon Harpham and three anonymous reviewers for their valuable inputs on the topic. DV is funded through the project CAP4GI by the Federal Ministry of Education and Research (BMBF), within the framework of the Strategy „Research for Sustainability" (FONA, [www.fona.de/en](http://www.fona.de/en)) as part of its Social-Ecological Research funding priority, funding no. 01UT2102A. Responsibility for the content of this publication lies with the authors. DV and GP gratefully acknowledge the support of iDiv, funded by the German Research Foundation (DFG–FZT 118, 202548816). SMF gratefully acknowledges funding received from the German Research Foundation (DFG; project ForcTrait).

## Author contributions

DV and SMF conceived the idea for the review and developed the figures; DV led the writing of the manuscript; all authors contributed critically to the drafts and gave final approval for publication.

## References

- Abelson, H., Sussman, G. J., & Sussman, J. (1996). *Structure and interpretation of computer programs* (2. ed). MIT Press.  
OCLC: 34576857.

- Armstrong McKay, D. I., Staal, A., Abrams, J. F., Winkelmann, R., Sakschewski, B., Loriani, S., Fetzner, I., Cornell, S. E., Rockström, J., & Lenton, T. M. (2022). Exceeding 1.5°C global warming could trigger multiple climate tipping points. *Science*, 377(6611), eabn7950. <https://doi.org/10.1126/science.abn7950>
- Balaban, G., Grytten, I., Rand, K. D., Scheffer, L., & Sandve, G. K. (2021). Ten simple rules for quick and dirty scientific programming. *PLOS Computational Biology*, 17(3), e1008549. <https://doi.org/10.1371/journal.pcbi.1008549>
- Barton, C. M., Lee, A., Janssen, M. A., Porter, C., Greenberg, J., Swantek, L., Frank, K., Chen, M., & Jagers, H. R. A. (2022). How to make models more useful. *Proceedings of the National Academy of Sciences*, 119(35), 4.
- Beck, F., & Diehl, S. (2011). On the congruence of modularity and code coupling. *Proceedings of the 19th ACM SIGSOFT Symposium and the 13th European Conference on Foundations of Software Engineering*, 354–364. <https://doi.org/10.1145/2025113.2025162>
- Belete, G. F., Voinov, A., & Laniak, G. F. (2017). An overview of the model integration process: From pre-integration assessment to testing. *Environmental Modelling & Software*, 87, 49–63. <https://doi.org/10.1016/j.envsoft.2016.10.013>
- Bell, A. R., Robinson, D. T., Malik, A., & Dewal, S. (2015). Modular ABM development for improved dissemination and training. *Environmental Modelling & Software*, 73, 189–200. <https://doi.org/10.1016/j.envsoft.2015.07.016>
- Berger, U., Bell, A., Barton, C. M., Chappin, E., Dreßler, G., Filatova, T., Fronville, T., Lee, A., van Loon, E., Lorscheid, I., Meyer, M., Müller, B., Piou, C., Radchuk, V., Roxburgh, N., Schüller, L., Troost, C., Wijermans, N., Williams, T. G., . . . Grimm, V. (2024). Towards reusable building blocks for agent-based modelling and theory development. *Environmental Modelling & Software*, 175, 106003. <https://doi.org/10.1016/j.envsoft.2024.106003>
- Bocedi, G., Palmer, S. C. F., Malchow, A.-K., Zurell, D., Watts, K., & Travis, J. M. J. (2021). RangeShifter 2.0: An extended and enhanced platform for modelling spatial eco-evolutionary dynamics and species’ responses to environmental changes. *Ecography*, 44(10), 1453–1462. <https://doi.org/10.1111/ecog.05687>
- Bohn, F. J., Frank, K., & Huth, A. (2014). Of climate and its resulting tree growth: Simulating the productivity of temperate forests. *Ecological Modelling*, 278, 9–17. <https://doi.org/10.1016/j.ecolmodel.2014.01.021>
- Brandmeyer, J. E., & Karimi, H. A. (2000). Coupling methodologies for environmental models. *Environmental Modelling & Software*, 15(5), 479–488. [https://doi.org/10.1016/S1364-8152\(00\)00027-X](https://doi.org/10.1016/S1364-8152(00)00027-X)

- Brooks, F. (1986). No Silver Bullet – Essence and Accident in Software Engineering. In H.-J. Kugler (Ed.), *Proceedings of the IFIP Tenth World Computing Conference* (pp. 1069–1076). Elsevier Science B.V.
- Brown, A., & Wilson, G. (Eds.). (2011). *The Architecture of Open Source Applications*. Creative Commons.  
OCLC: 936178393.
- Bulatewicz, T., Yang, X., Peterson, J. M., Staggenborg, S., Welch, S. M., & Steward, D. R. (2010). Accessible integration of agriculture, groundwater, and economic models using the Open Modeling Interface (OpenMI): Methodology and initial results. *Hydrol. Earth Syst. Sci.*, 14.
- Cabral, J. S., Mendoza-Ponce, A., da Silva, A. P., Oberpriller, J., Mimet, A., Kieslinger, J., Berger, T., Blechschmidt, J., Brönnner, M., Classen, A., Fallert, S., Hartig, F., Hof, C., Hoffmann, M., Knoke, T., Krause, A., Lewerentz, A., Pohle, P., Raeder, U., . . . Zurell, D. (2023). The road to integrate climate change projections with regional land-use–biodiversity models. *People and Nature*, n/a(n/a). <https://doi.org/10.1002/pan3.10472>
- Cabral, J. S., Valente, L., & Hartig, F. (2017). Mechanistic simulation models in macroecology and biogeography: State-of-art and prospects. *Ecography*, 40(2), 267–280. <https://doi.org/10.1111/ecog.02480>
- Churavy, V., Godoy, W. F., Bauer, C., Ranocha, H., Schlottke-Lakemper, M., Räss, L., Blaschke, J., Giordano, M., Schnetter, E., Omlin, S., Vetter, J. S., & Edelman, A. (2022, November 10). *Bridging HPC Communities through the Julia Programming Language*. arXiv: 2211.02740 [cs]. <https://doi.org/10.48550/arXiv.2211.02740>
- Cohen, J., Katz, D. S., Barker, M., Hong, N. C., Haines, R., & Jay, C. (2021). The Four Pillars of Research Software Engineering. *IEEE Software*, 38(1), 97–105. <https://doi.org/10.1109/MS.2020.2973362>
- David, O., Ascough, J. C., Lloyd, W., Green, T. R., Rojas, K. W., Leavesley, G. H., & Ahuja, L. R. (2013). A software engineering perspective on environmental modeling framework design: The Object Modeling System. *Environmental Modelling & Software*, 39, 201–213. <https://doi.org/10.1016/j.envsoft.2012.03.006>
- DeAngelis, D. L., & Grimm, V. (2014). Individual-based models in ecology after four decades. *F1000prime reports*, 6, 39. <https://doi.org/10.12703/P6-39>
- Dijkstra, E. W. (1972). The humble programmer. *Communications of the ACM*, 15(10), 859–866. <https://doi.org/10.1145/355604.361591>

- Dislich, C., & Huth, A. (2012). Modelling the impact of shallow landslides on forest structure in tropical montane forests. *Ecological Modelling*, 239, 40–53. <https://doi.org/10.1016/j.ecolmodel.2012.04.016>
- Edwards, P. N. (2011). History of climate modeling. *WIREs Climate Change*, 2(1), 128–139. <https://doi.org/10.1002/wcc.95>
- Enders, A., Martre, P., Raynal, H., Athanasiadis, I., Donatelli, M., Fumagalli, D., Holzworth, D., Stöckle, C., & Hoogenboom, G. (2018). Agricultural Model Exchange Initiative (AMEI), 61. <https://scholarsarchive.byu.edu/iemssconference/2018/Stream-A/61>
- Evans, L. C., Sibly, R. M., Thorbek, P., Sims, I., Oliver, T. H., & Walters, R. J. (2019). Quantifying the effectiveness of agri-environment schemes for a grassland butterfly using individual-based models. *Ecological Modelling*, 411, 108798. <https://doi.org/10.1016/j.ecolmodel.2019.108798>
- Eyring, V., Bony, S., Meehl, G. A., Senior, C. A., Stevens, B., Stouffer, R. J., & Taylor, K. E. (2016). Overview of the Coupled Model Intercomparison Project Phase 6 (CMIP6) experimental design and organization. *Geoscientific Model Development*, 9(5), 1937–1958. <https://doi.org/10.5194/gmd-9-1937-2016>
- Farahbakhsh, I., Bauch, C. T., & Anand, M. (2022). Modelling coupled human–environment complexity for the future of the biosphere: Strengths, gaps and promising directions. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 377(1857), 20210382. <https://doi.org/10.1098/rstb.2021.0382>
- Farrell, K. J., & Carey, C. C. (2018). Power, pitfalls, and potential for integrating computational literacy into undergraduate ecology courses. *Ecology and Evolution*, 8(16), 7744–7751. <https://doi.org/10.1002/ece3.4363>
- Fer, I., Gardella, A. K., Shiklomanov, A. N., Campbell, E. E., Cowdery, E. M., De Kauwe, M. G., Desai, A., Duveneck, M. J., Fisher, J. B., Haynes, K. D., Hoffman, F. M., Johnston, M. R., Kooper, R., LeBauer, D. S., Mantooth, J., Parton, W. J., Poulter, B., Quaife, T., Raiho, A., . . . Dietze, M. C. (2021). Beyond ecosystem modeling: A roadmap to community cyberinfrastructure for ecological data-model integration. *Global Change Biology*, 27(1), 13–26. <https://doi.org/10.1111/gcb.15409>
- Filazzola, A., & Lortie, C. (2022). A call for clean code to effectively communicate science. *Methods in Ecology and Evolution*, n/a(n/a). <https://doi.org/10.1111/2041-210X.13961>

- 796 Fischer, R. (2021). The Long-Term Consequences of Forest Fires on the Carbon Fluxes  
797 of a Tropical Forest in Africa. *Applied Sciences*, 11(10), 4696. [https://doi.org/](https://doi.org/10.3390/app11104696)  
798 10.3390/app11104696
- 799 Fischer, R., Bohn, F., Dantas De Paula, M., Dislich, C., Groeneveld, J., Gutiérrez, A. G.,  
800 Kazmierczak, M., Knapp, N., Lehmann, S., Paulick, S., Pütz, S., Rödig, E.,  
801 Taubert, F., Köhler, P., & Huth, A. (2016). Lessons learned from applying a  
802 forest gap model to understand ecosystem and carbon dynamics of complex trop-  
803 ical forests. *Ecological Modelling*, 326, 124–133. [https://doi.org/10.1016/j.](https://doi.org/10.1016/j.ecolmodel.2015.11.018)  
804 ecolmodel.2015.11.018
- 805 Fust, P., & Schlecht, E. (2018). Integrating spatio-temporal variation in resource availabil-  
806 ity and herbivore movements into rangeland management: RaMDry—An agent-  
807 based model on livestock feeding ecology in a dynamic, heterogeneous, semi-arid  
808 environment. *Ecological Modelling*, 369, 13–41. [https://doi.org/10.1016/j.](https://doi.org/10.1016/j.ecolmodel.2017.10.017)  
809 ecolmodel.2017.10.017
- 810 Gregersen, J. B., Gijsbers, P. J. A., & Westen, S. J. P. (2007). OpenMI: Open modelling  
811 interface. *Journal of Hydroinformatics*, 9(3), 175–191. [https://doi.org/10.2166/](https://doi.org/10.2166/hydro.2007.023)  
812 hydro.2007.023
- 813 Grimm, V., Ayllón, D., & Railsback, S. F. (2017). Next-Generation Individual-Based  
814 Models Integrate Biodiversity and Ecosystems: Yes We Can, and Yes We Must.  
815 *Ecosystems*, 20(2), 229–236. <https://doi.org/10.1007/s10021-016-0071-2>
- 816 Grimm, V., Johnston, A. S. A., Thulke, H.-H., Forbes, V. E., & Thorbek, P. (2020).  
817 Three questions to ask before using model outputs for decision support. *Nature*  
818 *Communications*, 11(1), 4959. <https://doi.org/10.1038/s41467-020-17785-2>
- 819 Grimm, V., & Railsback, S. F. (2005). *Individual-based Modeling and Ecology*. Princeton  
820 University Press.
- 821 Grimm, V., Railsback, S. F., Vincenot, C. E., Berger, U., Gallagher, C., DeAngelis, D. L.,  
822 Edmonds, B., Ge, J., Giske, J., Groeneveld, J., Johnston, A. S. A., Milles, A.,  
823 Nabe-Nielsen, J., Polhill, J. G., Radchuk, V., Rohwäder, M.-S., Stillman, R. A.,  
824 Thiele, J. C., & Ayllón, D. (2020). The ODD Protocol for Describing Agent-Based  
825 and Other Simulation Models: A Second Update to Improve Clarity, Replication,  
826 and Structural Realism. *Journal of Artificial Societies and Social Simulation*,  
827 23(2), 7. <https://doi.org/10.18564/jasss.4259>
- 828 Guillem, E., Murray-Rust, D., Robinson, D., Barnes, A., & Rounsevell, M. (2015). Mod-  
829 elling farmer decision-making to anticipate tradeoffs between provisioning ecosys-  
830 tem services and biodiversity. *Agricultural Systems*, 137, 12–23. [https://doi.org/](https://doi.org/10.1016/j.agry.2015.03.006)  
831 10.1016/j.agry.2015.03.006



- 832 Gutiérrez, A. G., Armesto, J. J., Díaz, M. F., & Huth, A. (2014). Increased Drought  
833 Impacts on Temperate Rainforests from Southern South America: Results of  
834 a Process-Based, Dynamic Forest Model (B. Hérault, Ed.). *PLoS ONE*, 9(7),  
835 e103226. <https://doi.org/10.1371/journal.pone.0103226>
- 836 Hagen, O., Flück, B., Fopp, F., Cabral, J. S., Hartig, F., Pontarp, M., Rangel, T. F., &  
837 Pellissier, L. (2021). Gen3sis: A general engine for eco-evolutionary simulations  
838 of the processes that shape Earth’s biodiversity. *PLOS Biology*, 19(7), e3001340.  
839 <https://doi.org/10.1371/journal.pbio.3001340>
- 840 Harfoot, M. B. J., Newbold, T., Tittensor, D. P., Emmott, S., Hutton, J., Lyutsarev,  
841 V., Smith, M. J., Scharlemann, J. P. W., & Purves, D. W. (2014). Emergent  
842 Global Patterns of Ecosystem Structure and Function from a Mechanistic General  
843 Ecosystem Model. *PLOS Biology*, 12(4), e1001841. [https://doi.org/10.1371/](https://doi.org/10.1371/journal.pbio.1001841)  
844 [journal.pbio.1001841](https://doi.org/10.1371/journal.pbio.1001841)
- 845 Harfoot, M. B. J., Tittensor, D. P., Newbold, T., McInerny, G., Smith, M. J., & Scharle-  
846 mann, J. P. W. (2014). Integrated assessment models for ecologists: The present  
847 and the future. *Global Ecology and Biogeography*, 23(2), 124–143. [https://doi.](https://doi.org/10.1111/geb.12100)  
848 [org/10.1111/geb.12100](https://doi.org/10.1111/geb.12100)
- 849 Harpham, Q., Hughes, A., & Moore, R. (2019). Introductory overview: The OpenMI 2.0  
850 standard for integrating numerical models. *Environmental Modelling & Software*,  
851 122, 104549. <https://doi.org/10.1016/j.envsoft.2019.104549>
- 852 Hasselbring, W., Carr, L., Hettrick, S., Packer, H., & Tiropanis, T. (2020). From FAIR  
853 research data toward FAIR and open research software. *it - Information Technol-*  
854 *ogy*, 62(1), 39–47. <https://doi.org/10.1515/itit-2019-0040>
- 855 Hill, C., DeLuca, C., Balaji, Suarez, M., & Da Silva, A. (2004). The architecture of the  
856 earth system modeling framework. *Computing in Science & Engineering*, 6(1),  
857 18–28. <https://doi.org/10.1109/MCISE.2004.1255817>
- 858 Hoeks, S., Tucker, M. A., Huijbregts, M. A. J., Harfoot, M. B. J., Bithell, M., & Santini, L.  
859 (2021). MadingleyR: An R package for mechanistic ecosystem modelling. *Global*  
860 *Ecology and Biogeography*, 30(9), 1922–1933. <https://doi.org/10.1111/geb.13354>
- 861 Holzworth, D. P., Huth, N. I., & deVoil, P. G. (2011). Simple software processes and  
862 tests improve the reliability and usefulness of a model. *Environmental Modelling*  
863 *& Software*, 26(4), 510–516. <https://doi.org/10.1016/j.envsoft.2010.10.014>
- 864 IPBES. (2016). *The Methodological Assessment Report on Scenarios and Models of Bio-*  
865 *diversity and Ecosystem Services*. ecretariat of the Intergovernmental Science-  
866 Policy Platform on Biodiversity and Ecosystem Services. Bonn, Germany. Re-

trieved March 4, 2022, from [https://ipbes.net/sites/default/files/downloads/pdf/2016.methodological\\_assessment\\_report\\_scenarios\\_models.pdf](https://ipbes.net/sites/default/files/downloads/pdf/2016.methodological_assessment_report_scenarios_models.pdf)

Janssen, M. A., Alessa, L. N., Barton, M., Bergin, S., & Lee, A. (2008). Towards a Community Framework for Agent-Based Modelling. *Journal of Artificial Societies and Social Simulation*, 11(26), 1–13. <https://www.jasss.org/11/2/6/6.pdf>

Janssen, M. A., Pritchard, C., & Lee, A. (2020). On code sharing and model documentation of published individual and agent-based models. *Environmental Modelling & Software*, 134, 104873. <https://doi.org/10.1016/j.envsoft.2020.104873>

Janssen, S., Athanasiadis, I. N., Bezlepkin, I., Knapen, R., Li, H., Domínguez, I. P., Rizzoli, A. E., & van Ittersum, M. K. (2011). Linking models for assessing agricultural land use change. *Computers and Electronics in Agriculture*, 76(2), 148–160. <https://doi.org/10.1016/j.compag.2010.10.011>

Jetz, W., McGeoch, M. A., Guralnick, R., Ferrier, S., Beck, J., Costello, M. J., Fernandez, M., Geller, G. N., Keil, P., Merow, C., Meyer, C., Muller-Karger, F. E., Pereira, H. M., Regan, E. C., Schmeller, D. S., & Turak, E. (2019). Essential biodiversity variables for mapping and monitoring species populations. *Nature Ecology & Evolution*, 3(4), 539–551. <https://doi.org/10.1038/s41559-019-0826-1>

Johanson, A., & Hasselbring, W. (2018). Software Engineering for Computational Science: Past, Present, Future. *Computing in Science & Engineering*, 20(2), 90–109. <https://doi.org/10.1109/MCSE.2018.021651343>

Kim, H., Rosa, I. M. D., Alkemade, R., Leadley, P., Hurtt, G., Popp, A., van Vuuren, D. P., Anthoni, P., Arneth, A., Baisero, D., Caton, E., Chaplin-Kramer, R., Chini, L., De Palma, A., Di Fulvio, F., Di Marco, M., Espinoza, F., Ferrier, S., Fujimori, S., ... Pereira, H. M. (2018). A protocol for an intercomparison of biodiversity and ecosystem services models using harmonized land-use and climate scenarios. *Geoscientific Model Development*. <https://doi.org/10.5194/gmd-2018-115>

Knapen, R., Janssen, S., Roosenschoon, O., Verweij, P., de Winter, W., Uiterwijk, M., & Wien, J.-E. (2013). Evaluating OpenMI as a model integration platform across disciplines. *Environmental Modelling & Software*, 39, 274–282. <https://doi.org/10.1016/j.envsoft.2012.06.011>

Köhler, P., & Huth, A. (1998). The effects of tree species grouping in tropical rainforest modelling: Simulations with the individual-based model Formind. *Ecological Modelling*, 109(3), 301–321. [https://doi.org/10.1016/S0304-3800\(98\)00066-0](https://doi.org/10.1016/S0304-3800(98)00066-0)

Lange, M., Müller, S., Fischer, T., König, S., Rojas, J. J. L., Kelbling, M., Thober, S., & Attinger, S. (2023). *FINAM* (Version 0.4). Leipzig, Germany. Retrieved June 12, 2023, from <https://finam.pages.ufz.de/>

- 903 Le, Q. B., Park, S. J., Vlek, P. L., & Cremers, A. B. (2008). Land-Use Dynamic Simulator  
 904 (LUDAS): A multi-agent system model for simulating spatio-temporal dynamics  
 905 of coupled human–landscape system. I. Structure and theoretical specification.  
 906 *Ecological Informatics*, 3(2), 135–153. [https://doi.org/10.1016/j.ecoinf.2008.04.](https://doi.org/10.1016/j.ecoinf.2008.04.003)  
 907 003
- 908 Lee, B. D. (2018). Ten simple rules for documenting scientific software. *PLOS Computa-*  
 909 *tional Biology*, 14(12), e1006561. <https://doi.org/10.1371/journal.pcbi.1006561>
- 910 Lee, J.-Y., Marotzke, J., Bala, G., Cao, L., Corti, S., Dunne, J., Engelbrecht, F., Fischer,  
 911 E., Fyfe, J., Jones, C., Maycock, A., Mutemi, J., Ndiaye, O., Panickal, S., &  
 912 Zhou, T. (2021). Future Global Climate: Scenario-based Projections and Near-  
 913 term Information. In V. Masson-Delmotte, P. Zhai, A. Pirani, S. Connors, C.  
 914 Péan, S. Berger, N. Caud, Y. Chen, L. Goldfarb, M. Gomis, M. Huang, K. Leitzell,  
 915 E. Lonnoy, J. Matthews, T. Maycock, T. Waterfield, O. Yelekci, R. Yu & B.  
 916 Zhou (Eds.), *Climate Change 2021: The Physical Science Basis. Contribution of*  
 917 *Working Group I to the Sixth Assessment Report of the Intergovernmental Panel*  
 918 *on Climate Change* (pp. 553–672). Cambridge University Press.  
 919 <https://doi.org/10.1017/9781009157896.006>.
- 920 Lehmann, S., & Huth, A. (2015). Fast calibration of a dynamic vegetation model with  
 921 minimum observation data. *Ecological Modelling*, 301, 98–105. [https://doi.org/](https://doi.org/10.1016/j.ecolmodel.2015.01.013)  
 922 10.1016/j.ecolmodel.2015.01.013
- 923 Leidinger, L., Vedder, D., & Cabral, J. S. (2021). Temporal environmental variation may  
 924 impose differential selection on both genomic and ecological traits. *Oikos*, 130(7),  
 925 1100–1115. <https://doi.org/10.1111/oik.08172>
- 926 Lippe, M., Bithell, M., Gotts, N., Natalini, D., Barbrook-Johnson, P., Giupponi, C.,  
 927 Hallier, M., Hofstede, G. J., Le Page, C., Matthews, R. B., Schlüter, M., Smith,  
 928 P., Teglio, A., & Thellmann, K. (2019). Using agent-based modelling to simulate  
 929 social-ecological systems across scales. *GeoInformatica*, 23(2), 269–298. [https:](https://doi.org/10.1007/s10707-018-00337-8)  
 930 [//doi.org/10.1007/s10707-018-00337-8](https://doi.org/10.1007/s10707-018-00337-8)
- 931 Lorscheid, I., & Meyer, M. (2016). Divide and conquer: Configuring submodels for valid  
 932 and efficient analyses of complex simulation models. *Ecological Modelling*, 326,  
 933 152–161. <https://doi.org/10.1016/j.ecolmodel.2015.11.013>
- 934 Maji, A. K., Gorenstein, L., & Lentner, G. (2020). Demystifying Python Package Instal-  
 935 lation with conda-env-mod. *2020 IEEE/ACM International Workshop on HPC*  
 936 *User Support Tools (HUST) and Workshop on Programming and Performance Vi-*  
 937 *sualization Tools (ProTools)*, 27–37. [https://doi.org/10.1109/HUSTProTools51951.](https://doi.org/10.1109/HUSTProTools51951.2020.00011)  
 938 2020.00011

- 939 Malawska, A., & Topping, C. J. (2018). Applying a biocomplexity approach to modelling  
940 farmer decision-making and land use impacts on wildlife (J. du Toit, Ed.). *Journal*  
941 *of Applied Ecology*, 55(3), 1445–1455. <https://doi.org/10.1111/1365-2664.13024>
- 942 Malawska, A., Topping, C. J., & Nielsen, H. Ø. (2014). Why do we need to integrate  
943 farmer decision making and wildlife models for policy evaluation? *Land Use Pol-*  
944 *icy*, 38, 732–740. <https://doi.org/10.1016/j.landusepol.2013.10.025>
- 945 Malchow, A.-K., Bocedi, G., Palmer, S. C. F., Travis, J. M. J., & Zurell, D. (2021).  
946 RangeShiftR: An R package for individual-based simulation of spatial eco-evolutionary  
947 dynamics and species’ responses to environmental changes. *Ecography*, 44(10),  
948 1443–1452. <https://doi.org/10.1111/ecog.05689>
- 949 Manabe, S. (2019). Role of greenhouse gas in climate change. *Tellus A: Dynamic Mete-*  
950 *orology and Oceanography*, 71(1), 1620078. [https://doi.org/10.1080/16000870.](https://doi.org/10.1080/16000870.2019.1620078)  
951 2019.1620078
- 952 Martin, R. C. (Ed.). (2009). *Clean code: A handbook of agile software craftsmanship*.  
953 Prentice Hall.
- 954 Marwick, B., Boettiger, C., & Mullen, L. (2018). Packaging Data Analytical Work Repro-  
955 ducibly Using R (and Friends). *The American Statistician*, 72(1), 80–88. <https://doi.org/10.1080/00031305.2017.1375986>
- 956 McConnell, S. (2004). *Code Complete* (2nd ed). Microsoft Press.
- 957 McIntire, E. J. B., Chubaty, A. M., Cumming, S. G., Andison, D., Barros, C., Boisvenue,  
958 C., Haché, S., Luo, Y., Micheletti, T., & Stewart, F. E. C. (2022). PERFICT:  
959 A Re-imagined foundation for predictive ecology. *Ecology Letters*, 25(6), 1345–  
960 1351. <https://doi.org/10.1111/ele.13994>
- 961 Mislan, K. A. S., Heer, J. M., & White, E. P. (2016). Elevating The Status of Code in  
962 Ecology. *Trends in Ecology & Evolution*, 31(1), 4–7. <https://doi.org/10.1016/j.jtree.2015.11.006>
- 963 Nowogrodzki, A. (2019). Tips for Open-Source Software Support. *Nature*, 571(7763),  
964 133–134. <https://doi.org/10.1038/d41586-019-02046-0>
- 965 O’Sullivan, D., Evans, T., Manson, S., Metcalf, S., Liggmann-Zielinska, A., & Bone, C.  
966 (2016). Strategic directions for agent-based modeling: Avoiding the YAAWN syn-  
967 drome. *Journal of Land Use Science*, 11(2), 177–187. <https://doi.org/10.1080/1747423X.2015.1030463>
- 968 Pan, H., & Chen, Z. (2021). Crop Growth Modeling and Yield Forecasting. In L. Di  
969 & B. Üstündağ (Eds.), *Agro-geoinformatics: Theory and Practice* (pp. 205–220).  
970 Springer International Publishing. [https://doi.org/10.1007/978-3-030-66387-](https://doi.org/10.1007/978-3-030-66387-2_11)  
971 2\_11

975 Perez-Riverol, Y., Gatto, L., Wang, R., Sachsenberg, T., Uszkoreit, J., Leprevost, F. d. V.,  
976 Fufezan, C., Ternent, T., Eglén, S. J., Katz, D. S., Pollard, T. J., Kononov, A.,  
977 Flight, R. M., Blin, K., & Vizcaíno, J. A. (2016). Ten Simple Rules for Taking  
978 Advantage of Git and GitHub. *PLOS Computational Biology*, 12(7), e1004947.  
979 <https://doi.org/10.1371/journal.pcbi.1004947>

980 Pilowsky, J. A., Colwell, R. K., Rahbek, C., & Fordham, D. A. (2022). Process-explicit  
981 models reveal the structure and dynamics of biodiversity patterns. *Science Ad-  
982 vances*, 8(31), eabj2271. <https://doi.org/10.1126/sciadv.abj2271>

983 Piórr, A., Ungaro, F., Ciancaglini, A., Happe, K., Sahrbacher, A., Sattler, C., Uthes,  
984 S., & Zander, P. (2009). Integrated assessment of future CAP policies: Land use  
985 changes, spatial patterns and targeting. *Environmental Science & Policy*, 12(8),  
986 1122–1136. <https://doi.org/10.1016/j.envsci.2009.01.001>

987 Pörtner, H.-O., Scholes, R. J., Agard, J., Archer, E., Arneth, A., Bai, X., Barnes, D.,  
988 Burrows, M., Chan, L., Cheung, W. L. (, Diamond, S., Donatti, C., Duarte,  
989 C., Eisenhauer, N., Foden, W., Gasalla, M. A., Handa, C., Hickler, T., Hoegh-  
990 Guldberg, O., . . . Ngo, H. (2021, June 24). *Scientific outcome of the IPBES-IPCC  
991 co-sponsored workshop on biodiversity and climate change*. IPBES secretariat.  
992 Bonn, Germany. <https://doi.org/10.5281/zenodo.5101125>

993 Prabhu, P., Jablin, T. B., Raman, A., Zhang, Y., Huang, J., Kim, H., Johnson, N. P.,  
994 Liu, F., Ghosh, S., Beard, S., Oh, T., Zoufaly, M., Walker, D., & August, D. I.  
995 (2011). A survey of the practice of computational science. *State of the Practice  
996 Reports*, 1–12. <https://doi.org/10.1145/2063348.2063374>

997 Pütz, S., Groeneveld, J., Alves, L., Metzger, J., & Huth, A. (2011). Fragmentation drives  
998 tropical forest fragments to early successional states: A modelling study for Brazil-  
999 ian Atlantic forests. *Ecological Modelling*, 222(12), 1986–1997. <https://doi.org/10.1016/j.ecolmodel.2011.03.038>

1000

1001 Ram, K., Boettiger, C., Chamberlain, S., Ross, N., Salmon, M., & Butland, S. (2019). A  
1002 Community of Practice Around Peer Review for Long-Term Research Software  
1003 Sustainability. *Computing in Science Engineering*, 21(2), 59–65. <https://doi.org/10.1109/MCSE.2018.2882753>

1004

1005 Reidsma, P., Janssen, S., Jansen, J., & van Ittersum, M. K. (2018). On the development  
1006 and use of farm models for policy impact assessment in the European Union – A  
1007 review. *Agricultural Systems*, 159, 111–125. [https://doi.org/10.1016/j.agsy.2017.  
1008 10.012](https://doi.org/10.1016/j.agsy.2017.10.012)

1009 Robinson, D. T., Di Vittorio, A., Alexander, P., Arneth, A., Barton, C. M., Brown,  
1010 D. G., Kettner, A., Lemmen, C., O’Neill, B. C., Janssen, M., Pugh, T. A. M.,

- 1011 Rabin, S. S., Rounsevell, M., Syvitski, J. P., Ullah, I., & Verburg, P. H. (2018).  
 1012 Modelling feedbacks between human and natural processes in the land system.  
 1013 *Earth System Dynamics*, 9(2), 895–914. <https://doi.org/10.5194/esd-9-895-2018>
- 1014 Rollins, N. D., Barton, C. M., Bergin, S., Janssen, M. A., & Lee, A. (2014). A Compu-  
 1015 tational Model Library for publishing model documentation and code. *Environ-*  
 1016 *mental Modelling & Software*, 61, 59–64. [https://doi.org/10.1016/j.envsoft.2014.](https://doi.org/10.1016/j.envsoft.2014.06.022)  
 1017 06.022
- 1018 Romero-Mujalli, D., Jeltsch, F., & Tiedemann, R. (2019). Individual-based modeling  
 1019 of eco-evolutionary dynamics: State of the art and future directions. *Regional*  
 1020 *Environmental Change*, 19(1), 1–12. <https://doi.org/10.1007/s10113-018-1406-7>
- 1021 Ropella, G. E., Railsback, S. F., & Jackson, S. K. (2002). Software Engineering Consid-  
 1022 erations for Individual-Based Models. *Natural Resource Modeling*, 15(1), 5–22.  
 1023 <https://doi.org/10.1111/j.1939-7445.2002.tb00077.x>
- 1024 Rosenzweig, C., Jones, J. W., Hatfield, J. L., Ruane, A. C., Boote, K. J., Thorburn, P.,  
 1025 Antle, J. M., Nelson, G. C., Porter, C., Janssen, S., Asseng, S., Basso, B., Ewert,  
 1026 F., Wallach, D., Baigorria, G., & Winter, J. M. (2013). The Agricultural Model  
 1027 Intercomparison and Improvement Project (AgMIP): Protocols and pilot studies.  
 1028 *Agricultural and Forest Meteorology*, 170, 166–182. [https://doi.org/10.1016/j.](https://doi.org/10.1016/j.agrformet.2012.09.011)  
 1029 agrformet.2012.09.011
- 1030 Rosenzweig, C., Arnell, N. W., Ebi, K. L., Lotze-Campen, H., Raes, F., Rapley, C.,  
 1031 Smith, M. S., Cramer, W., Frieler, K., Reyer, C. P. O., Schewe, J., van Vuuren,  
 1032 D., & Warszawski, L. (2017). Assessing inter-sectoral climate change risks: The  
 1033 role of ISIMIP. *Environmental Research Letters*, 12(1), 010301. [https://doi.org/](https://doi.org/10.1088/1748-9326/12/1/010301)  
 1034 10.1088/1748-9326/12/1/010301
- 1035 Samaniego, L., Kumar, R., & Attinger, S. (2010). Multiscale parameter regionalization of  
 1036 a grid-based hydrologic model at the mesoscale: MULTISCALE PARAMETER  
 1037 REGIONALIZATION. *Water Resources Research*, 46(5). [https://doi.org/10.](https://doi.org/10.1029/2008WR007327)  
 1038 1029/2008WR007327
- 1039 Sanders, R., & Kelly, D. (2008). Dealing with Risk in Scientific Software Development.  
 1040 *IEEE Software*, 25(4), 21–28. <https://doi.org/10.1109/MS.2008.84>
- 1041 Scheller, R. M., Sturtevant, B. R., Gustafson, E. J., Ward, B. C., & Mladenoff, D. J.  
 1042 (2010). Increasing the reliability of ecological models using modern software en-  
 1043 gineering techniques. *Frontiers in Ecology and the Environment*, 8(5), 253–260.  
 1044 <https://doi.org/10.1890/080141>
- 1045 Schmidt, A., Necpalova, M., Zimmermann, A., Mann, S., Six, J., & Mack, G. (2017).  
 1046 Direct and Indirect Economic Incentives to Mitigate Nitrogen Surpluses: A Sen-

sitivity Analysis. *Journal of Artificial Societies and Social Simulation*, 20(4), 77.  
<https://doi.org/10.18564/jasss.3477>

Accepted: 2019-11-05T15:53:51Z.

Schouten, R., Vesk, P. A., & Kearney, M. R. (2020). Integrating dynamic plant growth models and microclimates for species distribution modelling. *Ecological Modelling*, 435, 109262. <https://doi.org/10.1016/j.ecolmodel.2020.109262>

Schreinemachers, P., & Berger, T. (2011). An agent-based simulation model of human–environment interactions in agricultural systems. *Environmental Modelling & Software*, 26(7), 845–859. <https://doi.org/10.1016/j.envsoft.2011.02.004>

Shrestha, N. K., Leta, O. T., De Fraine, B., Garcia-Armisen, T., Ouattara, N. K., Servais, P., van Griensven, A., & Bauwens, W. (2013). Modelling Escherichia coli dynamics in the river Zenne (Belgium) using an OpenMI based integrated model. *Journal of Hydroinformatics*, 16(2), 354–374. <https://doi.org/10.2166/hydro.2013.171>

Sibly, R. M., Grimm, V., Martin, B. T., Johnston, A. S. A., 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. *Methods in Ecology and Evolution*, 4(2), 151–161. <https://doi.org/10.1111/2041-210x.12002>

Sieger, C. S., & Hovestadt, T. (2021). The effect of landscape structure on the evolution of two alternative dispersal strategies. *Ecological Processes*, 10(1), 73. <https://doi.org/10.1186/s13717-021-00343-z>

Simon, R. N., & Fortin, D. (2020). Crop raiders in an ecological trap: Optimal foraging individual-based modeling quantifies the effect of alternate crops. *Ecological Applications*, 30(5), e02111. <https://doi.org/10.1002/eap.2111>

Stillman, R. A., Wood, K. A., & Goss-Custard, J. D. (2016). Deriving simple predictions from complex models to support environmental decision-making. *Ecological Modelling*, 326, 134–141. <https://doi.org/10.1016/j.ecolmodel.2015.04.014>

Sun, Z., Lorscheid, I., Millington, J. D., Lauf, S., Magliocca, N. R., Groeneveld, J., Balbi, S., Nolzen, H., Müller, B., Schulze, J., & Buchmann, C. M. (2016). Simple or complicated agent-based models? A complicated issue. *Environmental Modelling & Software*, 86, 56–67. <https://doi.org/10.1016/j.envsoft.2016.09.006>

Synes, N. W., Brown, C., Palmer, S. C. F., Bocedi, G., Osborne, P. E., Watts, K., Franklin, J., & Travis, J. M. J. (2019). Coupled land use and ecological models reveal emergence and feedbacks in socio-ecological systems. *Ecography*, 42(4), 814–825. <https://doi.org/10.1111/ecog.04039>

- 1082 Theurich, G., DeLuca, C., Campbell, T., Liu, F., Saint, K., Vertenstein, M., Chen, J.,  
1083 Oehmke, R., Doyle, J., Whitcomb, T., Wallcraft, A., Iredell, M., Black, T., Silva,  
1084 A. M. D., Clune, T., Ferraro, R., Li, P., Kelley, M., Aleinov, I., . . . Dunlap, R.  
1085 (2016). The Earth System Prediction Suite: Toward a Coordinated U.S. Modeling  
1086 Capability. *Bulletin of the American Meteorological Society*, 97(7), 1229–1247.  
1087 <https://doi.org/10.1175/BAMS-D-14-00164.1>
- 1088 Topping, C. J., Hansen, T. S., Jensen, T. S., Jepsen, J. U., Nikolajsen, F., & Odderskær,  
1089 P. (2003). ALMaSS, an agent-based model for animals in temperate European  
1090 landscapes. *Ecological Modelling*, 167(1), 65–82. [https://doi.org/10.1016/S0304-](https://doi.org/10.1016/S0304-3800(03)00173-X)  
1091 [3800\(03\)00173-X](https://doi.org/10.1016/S0304-3800(03)00173-X)
- 1092 Topping, C. J. (2011). Evaluation of wildlife management through organic farming. *Eco-*  
1093 *logical Engineering*, 37(12), 2009–2017. [https://doi.org/10.1016/j.ecoleng.2011.](https://doi.org/10.1016/j.ecoleng.2011.08.010)  
1094 [08.010](https://doi.org/10.1016/j.ecoleng.2011.08.010)
- 1095 Topping, C. J., Alrøe, H. F., Farrell, K. N., & Grimm, V. (2015). Per Aspera ad As-  
1096 tra: Through Complex Population Modeling to Predictive Theory. *The American*  
1097 *Naturalist*, 186(5), 669–674. <https://doi.org/10.1086/683181>
- 1098 Topping, C. J. (2022). *ALMaSS - the animal, landscape and man simulation system*.  
1099 Aarhus, Denmark. [https://gitlab.com/ChrisTopping/ALMaSS\\_all](https://gitlab.com/ChrisTopping/ALMaSS_all)
- 1100 Urban, M. C., Bocedi, G., Hendry, A. P., Mihoub, J.-B., Pe’er, G., Singer, A., Bridle,  
1101 J. R., Crozier, L. G., De Meester, L., Godsoe, W., Gonzalez, A., Hellmann, J. J.,  
1102 Holt, R. D., Huth, A., Johst, K., Krug, C. B., Leadley, P. W., Palmer, S. C. F.,  
1103 Pantel, J. H., . . . Travis, J. M. J. (2016). Improving the forecast for biodiversity  
1104 under climate change. *Science*, 353(6304), aad8466. [https://doi.org/10.1126/](https://doi.org/10.1126/science.aad8466)  
1105 [science.aad8466](https://doi.org/10.1126/science.aad8466)
- 1106 Urban, M. C., Travis, J. M. J., Zurell, D., Thompson, P. L., Synes, N. W., Scarpa, A.,  
1107 Peres-Neto, P. R., Malchow, A.-K., James, P. M. A., Gravel, D., De Meester,  
1108 L., Brown, C., Bocedi, G., Albert, C. H., Gonzalez, A., & Hendry, A. P. (2022).  
1109 Coding for Life: Designing a Platform for Projecting and Protecting Global Bio-  
1110 diversity. *BioScience*, 72(1), 91–104. <https://doi.org/10.1093/biosci/biab099>
- 1111 Vable, A. M., Diehl, S. F., & Glymour, M. M. (2021). Code Review as a Simple Trick  
1112 to Enhance Reproducibility, Accelerate Learning, and Improve the Quality of  
1113 Your Team’s Research. *American Journal of Epidemiology*, 190(10), 2172–2177.  
1114 <https://doi.org/10.1093/aje/kwab092>
- 1115 van Ittersum, M. K., Ewert, F., Heckeley, T., Wery, J., Alkan Olsson, J., Andersen,  
1116 E., Bezlepkina, I., Brouwer, F., Donatelli, M., Flichman, G., Olsson, L., Rizzoli,  
1117 A. E., van der Wal, T., Wien, J. E., & Wolf, J. (2008). Integrated assessment



1118 of agricultural systems – A component-based framework for the European Union  
1119 (SEAMLESS). *Agricultural Systems*, 96(1-3), 150–165. [https://doi.org/10.1016/](https://doi.org/10.1016/j.agry.2007.07.009)  
1120 [j.agry.2007.07.009](https://doi.org/10.1016/j.agry.2007.07.009)

1121 Vedder, D., Ankenbrand, M., & Cabral, J. S. (2021). Dealing with software complexity in  
1122 individual-based models. *Methods in Ecology and Evolution*, 12(12), 2324–2333.  
1123 <https://doi.org/10.1111/2041-210X.13716>

1124 Vedder, D., Leidinger, L., & Sarmiento Cabral, J. (2021). Propagule pressure and an inva-  
1125 sion syndrome determine invasion success in a plant community model. *Ecology*  
1126 *and Evolution*, 11(23), 17106–17116. <https://doi.org/10.1002/ece3.8348>

1127 Vedder, D., Lens, L., Martin, C. A., Pellikka, P., Adhikari, H., Heiskanen, J., Engler,  
1128 J. O., & Sarmiento Cabral, J. (2022). Hybridization may aid evolutionary rescue  
1129 of an endangered East African passerine. *Evolutionary Applications*, 15(7), 1177–  
1130 1188. <https://doi.org/10.1111/eva.13440>

1131 Vedder, D., Rakowski, J., Kolb, L., Theilen, G., Lakner, S., & Pe’er, G. (submitted).  
1132 Agent-based modelling of agricultural social-ecological systems neglects biodiver-  
1133 sity.

1134 Will, M., Dressler, G., Kreuer, D., Thulke, H.-H., Grêt-Regamey, A., & Müller, B. (2021).  
1135 How to make socio-environmental modelling more useful to support policy and  
1136 management? *People and Nature*, 00, 1–13. <https://doi.org/10.1002/pan3.10207>

1137 Wilson, G., Aruliah, D. A., Brown, C. T., Chue Hong, N. P., Davis, M., Guy, R. T.,  
1138 Haddock, S. H. D., Huff, K. D., Mitchell, I. M., Plumbley, M. D., Waugh, B.,  
1139 White, E. P., & Wilson, P. (2014). Best Practices for Scientific Computing. *PLoS*  
1140 *Biology*, 12(1), 1–7. <https://doi.org/10.1371/journal.pbio.1001745>