simecol: An Object-Oriented Framework for Ecological Modeling in **R**

Thomas Petzoldt
Technische Universität Dresden

Karsten Rinke
Universität Konstanz

Abstract

The **simecol** package provides an open structure to implement, simulate and share ecological models. A generalized object-oriented architecture improves readability and potential code re-use of models and makes **simecol**-models freely extendable and simple to use. The **simecol** package was implemented in the S4 class system of the programming language **R**. Reference applications, e.g. predator-prey models or grid models are provided which can be used as a starting point for own developments. Compact example applications and the complete code of an individual-based model of the water flea *Daphnia* document the efficient usage of **simecol** for various purposes in ecological modeling, e.g. scenario analysis, stochastic simulations and individual based population dynamics. Ecologists are encouraged to exploit the abilities of **simecol** to structure their work and to use **R** and object-oriented programming as a suitable medium for the distribution and share of ecological modeling code.

Note: A previous version of this introduction to the R package simecol has been published as Petzoldt and Rinke (2007) in the Journal of Statistical Software, `http://www.jstatsoft.org/v22/i09`. Please refer to the original publication when citing this work.

Keywords: ecological modeling, individual-based model, object-oriented programming (OOP), code-sharing, **R**.

1. Introduction

The **R** system with the underlying **S** programming language is well suited for the development, implementation and analysis of dynamic models. It is, in addition to data analysis, increasingly used for model simulations in many disciplines like pharmacology (Tornø *et al.* 2004), psychology (van der Maas *et al.* 2006), microbiology (Jensen *et al.* 2006), epidemiology (Hartley *et al.* 2006), ecology (Fussmann *et al.* 2003; Rinke and Vijverberg 2005; Levey *et al.* 2005) or econometrics (Cribari-Neto and Zarkos 1999; Zeileis *et al.* 2005). Existing applications already cover a range from small conceptual process and teaching models up to coupled hydrodynamic-ecological models (Rolinski *et al.* 2005). Small models can be implemented easily in pure **R** (Petzoldt 2003) or by means of the XML-based Systems Biology Markup Language SBML and the corresponding Bioconductor package (Radivoyevitch 2004). For more complex or computation intensive simulations **R** is primarily used as an environment for data management, simulation control and data analysis, while the model core may be implemented in other languages like C/C++, FORTRAN or JAVA.

This works perfectly at the extremes, but problems appear with medium-sized models. While larger modeling projects usually start with an extensive planning and design phase carried out by experienced people, small models can be implemented ad-hoc without problems in R from scratch or by modification of online help examples. On the other hand, medium-sized applications often start by extension of small examples up to ever increasing size and complexity. An adequate design period is often skipped and at the end of a modeling project no time remains for re-design or appropriate documentation. The resulting programs are necessarily ill-structured in most cases or at least exhibit a very special, proprietary design.

The situation is even worse in ecological modeling, because this discipline is broad, modeling strategies vary substantially and ecological modelers are very creative. Different families of models (e.g. statistical, differential equations, discrete event, individual-based, spatially explicit) are applied alone or in mixtures to different ecological systems (terrestrial, limnetic, marine) and scales (individuals, laboratory systems, lakes/rivers/forests, oceans, biosphere). Not enough that there is a Babel of programming languages and simulation systems, there is also a Babel of approaches. There are often cases where it seems to be necessary to understand the whole source code when one tries to modify only one single parameter value or to introduce a new equation and it is not seldom easier to re-write code from scratch than to reuse an existing one.

We aim to propose a possible way out of the dilemma, an open structure to implement and simulate ecological models. The R package **simecol** is provided to demonstrate the feasibility of this approach including a starter set of examples and utility functions to work with such models.

After giving a description of the design goals and the specification of the `simObj` class in Sections 2 and 3 we demonstrate basic use of the package in Section 4. The different mechanisms available to implement and simulate `simObj` models are explained in Section 5. A complete individual-based model is given in Section 6 to elucidate how to use and extend **simecol** in the modeling process. Finally, we discuss perspectives of R and **simecol** in ecological modeling as well as relations to other packages (Section 7).

2. Design goals

Our first goal is to provide a generalized architecture for the implementation of ecological models. Such a unified style, which can be considered as a template or prototype of model implementations, provides manifold advantages for a scientific community. The structured architecture will increase readability of the code by separating model equations from other code elements, e.g. for numerical techniques. This will enable ecological modellers to use R as a communication medium and allows to distribute model source code together with its documentation, e.g. as executable part of the "standard protocol for describing individual-based and agent-based models" suggested by Grimm *et al.* (2006).

We want to stress that we don not intend to establish yet another simulation system. Complete simulation systems are numerous and well-established for specified applications, e.g.

STELLA[1], Berkeley Madonna[2], VENSIM[3], EcoBeaker[4] or the GNU open source system ECOBAS (Benz *et al.* 2001). A comprehensive overview about software used in ecological modeling is given elsewhere e.g. at http://www.systemdynamics.org/ or Chapter 8 of Grimm and Railsback (2005). These simulation systems can be extremely effective for the specific class of applications they are intended for, but, they often lack the full power and flexibility of a programming language. In such cases, model frameworks or simulation libraries are commonly used to support one specific model family, e.g. PASCAL templates for ordinary differential and delay-differential equations (Gurney and Nisbet 1998), an object-oriented C++ framework like OSIRIS (Mooij and Boersma 1996) for individual-based models or the Objective C framework SWARM[5] for agent-based simulations.

An alternative approach is the use of high-level programming environments and matrix oriented languages like MATLAB[6] or R (R Development Core Team 2006). Such languages allow a more interactive development cycle, compared to compiled languages, and outweigh their performance handicap by efficient algorithms and compiled libraries for numerics and data management. Both openness and interactivity have made the R system a universal scripting interface for the free combination of a large diversity of applications in statistics and scientific computing.

The second design goal is to be as open as possible and to take advantage of the open philosophy of R. Users should be allowed to employ the full power of R's graphical, statistical and data management functions and to use arbitrary code written in R or compiled languages. The complete code of **simecol**-models should be published under a license that minimizes dependence from others and guarantees unrestricted use in science and education, including the possibility to be modified by others. Within this context, **simecol** is intended to provide a framework on the meta-level identifying structure-components of ecological simulation models.

Our third design goal is ease of use and simplicity. One of the main characteristics of programming languages like S and R is that users become programmers (Chambers 2000). Unfortunately, ecologists are commonly not well-trained in programming, which often hampers their application of models. Therefore, we aim to provide a software layer that bridges this gap and helps ecologists to work with models. In consequence, this means for **simecol** that simplicity of implementation is more important than efficiency. The system should support a broad level of user experience – in our case ecological models covering the whole range from teaching models to research applications.

From the perspective of a first time user it should be possible to run simulations without knowing too much about R and implementation details. A simulation of an ecological model should be as easy as fitting a linear model in R (see example in Section 3.3.1). A number of memorable "commands", i.e. a few essential but not overwhelmingly extensive generics for simulation, printing, plotting and data access, and utility functions accompany this package. Both the functions and also the simulation models should have meaningful defaults to enable new users to get almost immediate success and to enable experienced developers to structure their applications and to avoid unnecessary copy and paste (Mächler 2004).

---

[1] http://www.iseesystems.com/
[2] http://www.berkeleymadonna.com/
[3] http://www.vensim.com/
[4] http://www.ecobeaker.com/
[5] http://www.swarm.org/
[6] http://www.mathworks.com/

3. Approach

The approach follows directly from the design goals to provide (i) a standardized structure, (ii) open and reusable code and (iii) ease of use of "the model". It is almost self-evident to apply an object-oriented design, consisting of:

1. A general and extensible class description suitable for ecological simulation models that allows sub-classes for different model families and multiple instances (objects of class simObj) which can be used simultaneously without interference,

2. Generic functions which work on objects of these classes and behave differently depending on the model family they work with.

All equations, constants and data needed for one particular simulation should be included in the model object, with the exception of general and widely needed functions, e.g. numerical algorithms. In the following sections we first analyse what is generally needed and then describe the particular approach.

3.1. State space approach

Most ecological models can be formulated by means of a state space representation, known from statistics and control theory (Figure 1). This applies to dynamic (discrete resp. continuous) systems as well as to static, time independent systems when postulating that the latter case is a subset. A general description that is valid for both linear and nonlinear systems can be given as:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t), \mathbf{p}) \tag{1}$$

$$\mathbf{y}(t) = \mathbf{g}(t, \mathbf{x}(t), \mathbf{u}(t), \mathbf{p}) \tag{2}$$

where $\mathbf{x}$ is the state of the system and $\dot{\mathbf{x}}$ its first derivative, t the time, $\mathbf{u}(t)$ is the input vector (or vector of boundary conditions), and $\mathbf{y}$ is the output vector. The functions $\mathbf{f}$ and $\mathbf{g}$ are the state transition function and the observation function, respectively, which rely on a vector $\mathbf{p}$ of constant parameters.

A simulation of a dynamic system is obtained by applying a suitable numerical algorithm to the function $\mathbf{f}$. This algorithm can be a simple iteration or, when $\mathbf{f}$ is a system of ordinary differential equations, an appropriate ODE solver or a function giving an analytical solution.

Compared to the usual statistical models in R, ecological models are more diverse in their structure and exhibit tight relationships between procedural code (methods, equations) and data. Non-trivial ecological models are based on more or less modular building blocks (sub-models), which are either base equations or complex models themselves.

3.2. The simObj specification

In essence, what do we need to implement a not too narrow class of ecological models? We need self-contained objects derived from classes with suitable properties and methods (data slots and function slots) resulting from the state space description: state variables, model
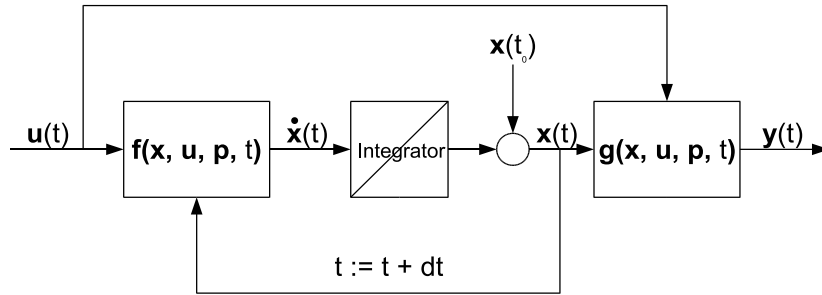
Figure 1: State space diagram of a dynamic system ($\mathbf{x}(t)$: state vector of the system, $\mathbf{x}(t_0)$ initial state, $\dot{\mathbf{x}}$: first derivative of the state vector, $\mathbf{u}$: input matrix, $\mathbf{y}(t)$: model output, $\mathbf{f}$ state transition function, $\mathbf{g}$ observation function, $\mathbf{p}$ constant parameters of $\mathbf{f}$ and $\mathbf{g}$), figure redrawn after Ludyk (1995), see also Bossel (1992) and Wolkenhauer *et al.* (2005).
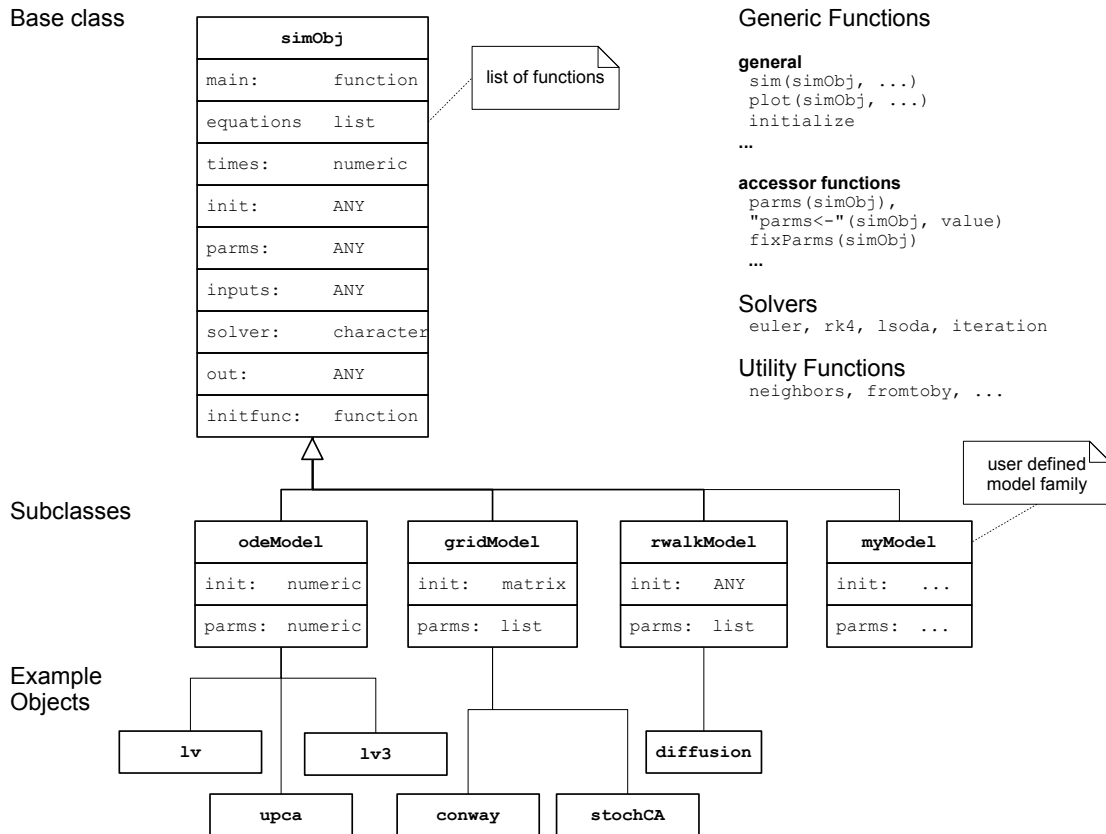

Figure 2: Class diagram of `simObj` and related classes. The subclasses and example model objects are provided as reference for user-defined and future extensions.

equations and algorithms, model parameters (constants), input values, time steps, the name of an appropriate numerical algorithm (solver), and an optional set of possibly nested sub-models (sub-equations). These parts are implemented as slots of the `simObj` class from which subclasses for different model families can inherit (Figure 2).

A small set of supporting functions is provided to work with these objects, namely:

- Generic functions for simulation, printing, plotting, slot manipulation (accessor functions) and object creation (`initialize` functions),

- Utility functions, e.g. neighborhood relations for cellular automata.

3.3. Generic functions

In the S4 class model of the S language methods are based on generic functions. They specify the behavior of a particular function, depending on the class of the function arguments (Chambers 2001). All generic functions in **simecol** are defined as default methods for the class `simObj` and specific methods exist if necessary for subclasses. If new subclasses are defined for additional model families by the user it may be necessary to create new methods that work with these user-defined data types and provide the required functionality.

Simulation

The core function to work with `simObj`ects is the generic function `sim(simObj, ...)`, which, for dynamic systems, simulates an initial value problem using the initial state, boundary conditions, equations and parameters stored in one particular `simObj` instance by calling the numerical algorithm referred by its name in the `solver` slot of `simObj`. Common for all versions of `sim` is the pass-back modification behavior, i.e. a modified version of the original `simObj` is returned with a newly added or updated slot `out` holding the simulation results:

```
R> library("simecol")
R> data(lv, package = "simecol")
R> lv <- sim(lv)
R> plot(lv)
R> o1 <- out(lv)
```

The functionality of `sim` can vary for different subclasses of `simObj` e.g. `odeModel`, `gridModel`, `rwalkModel`. This behavior results mainly from a different data structure of the state variables and the set of numerical algorithms that are adequate for a given family of ecological models. Whereas ODE models have a vector for state and a data frame for outputs, grid models may have a grid matrix for state and a list of grids (one grid per time step) as output, and finally, random walk models may have a list for the initial state of the particles and a list of lists for the output.

The returned `simObj` can be printed and plotted directly with appropriate functions, the simulation results can be extracted with `out` or the resulting `simObj` can be used in another simulation with modified data or functionality.

Accessor functions

Similar to the `out` function other accessor functions are available for all slots with (in opposite to `out`) not only read but also write access. These functions are used similarly like the base function `names` and work with the appropriate data structures, see help files for details. The functions allow to change either the whole content of the respective slot or to change single elements, e.g. parameter values, time steps or equations. For example, the following will change only the parameter value of `k1`:

```
R> parms(lv)
```

```
 k1  k2  k3
0.2 0.2 0.2
```

```
R> parms(lv)["k1"] <- 0.4
```

An entirely new parameter is added to the parameter vector via:

```
R> parms(lv)["a"] <- 1
R> parms(lv)
```

```
 k1  k2  k3   a
0.4 0.2 0.2 1.0
```

Elements can be deleted when a modified version of the parameter vector is assigned:

```
R> parms(lv) <- parms(lv)[-4]
R> parms(lv)
```

```
 k1  k2  k3
0.4 0.2 0.2
```

The behavior is analogous for all other slots with the exception of `out`, given that the correct data type for the respective slot (vector, list or matrix) is used.

In addition to the command line accessor functions, graphical Tcl/Tk versions exist (`fixParms`, `fixTimes`, `fixInit`), however, more complex data types cannot be handled yet by these functions.

Numerical algorithms

In order to simulate ecological models of various types, the appropriate numerical algorithms can be plugged into the `sim` function either by using an existing function, e.g. from this package, by imported solvers of package **odesolve** or by user-defined algorithms.

The algorithm used for one particular `simObj` is stored as character string in the `solver` slot of the object. User-defined algorithms have to provide interfaces (parameter line, output structure) and functionality (see below) that fit into the respective object specification and are compatible to the data structures of the particular class.

3.4. Utility functions

A few utility functions are provided for overcoming frequently occuring problems. However, it is not planned to overload **simecol** with numerous utilities as most of them are application-specific. Additional supporting functions should be written in the user workspace when they are needed or may be included in optional packages.

Interpolation

Dynamic systems often require interpolation of input data. This is particularly important for ODE solvers with automatic step size adjustment and there are cases where excessive interpolation outweighs the advantages of automatic step size determination.

The performance of linear approximation is crucial and we found that the performance of the respective functions from the **base** package can be increased if `approxfun` is used instead of `approx`, if matrices are used instead of data frames and if the number of data (nodes) in the inputs is limited to the essential minimum. In addition to this, two special versions `approxTime` and `approxTime1` provided by **simecol** may be useful, see the help file for details.

Neighborhood functions

The computation of neighborhood is time critical for cellular automata. Two `C++` functions, `eightneighbors` (direct neighbors) and `neighbors` (generalized neighborhood with arbitrary weight matrices) are provided for rectangular grids. The implementation of these functions is straightforward and may serve as a starting point for even more efficient solutions or other grid types, for example hexagonal or 3D grids.

Neighborhood functions can also be used for spatially explicit models. Models of this family commonly include both, an explicit spatial representation of organisms (in most cases with real-valued locations) and a grid-based representation of environmental factors (Dunning *et al.* 1995; Grimm and Railsback 2005).

3.5. Example models

A set of small ecological models is supplied with the package. These models are intended as a starting point for testing the package and for own developments. The models are provided in two versions, as binary objects in the data directory and in full source code in the directory "examples". The number of example models is intentionally limited and will grow only moderately in the future. In addition to this, ecological models which follow the `simObj` specification are well suited to be published and shared between scientists either as single code objects or in domain specific packages.

4. Two introductory examples

4.1. Cellular automaton

At the first level of experience, users can simply explore example models supplied with the package or provided by other users without carrying too much on implementation details.

```
CA <- new("gridModel",
    main = function(time, init, parms) {
        z      <- init
        nb     <- eightneighbors(z)
        pgen   <- 1 - (1 - parms$pbirth)^nb
        zgen   <- ifelse(z == 0 &
                    runif(z) < pgen, 1, 0)
        zsurv <- ifelse(z >= 1 &
                    runif(z) < (1 - parms$pdeath),
                    z + 1, 0)
        zgen + zsurv
    },
    parms  = list(pbirth = 0.02, pdeath = 0.01),
    times  = c(from = 1, to = 50, by = 1),
    init   = matrix(0, nrow = 40, ncol = 40),
    solver = "iteration"
)
init(CA)[18:22,18:22] <- 1
```
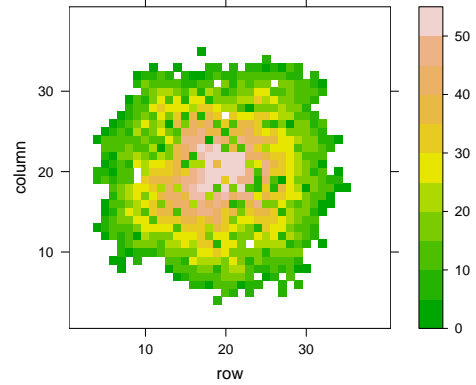

Figure 3: Stochastic cellular automaton, source code (left) and after 50 iterations (right).

They can be loaded with `source` from harddisk or the Internet, for example the stochastic cellular automaton shown in Figure 3:

```
R> library("simecol")
R> data(CA, package = "simecol")
R> CA <- sim(CA)
R> plot(CA)
```

Note, that the `sim` function uses pass-back modification, i.e. the result is the complete `simObj` with the model outputs inserted. The advantage is that the resulting `simObj` is consistent, i.e. the model output corresponds to the equations, parameters and other settings of the `simObj`. Now, the settings may be inspected and changed, e.g. the number of time steps:

```
R> times(CA)
R> times(CA) <- c(to = 100)
R> CA <- sim(CA)
R> plot(CA)
```

4.2. Predator-prey model

A second built-in demonstration example of **simecol**, is the elementary Lotka-Volterra predator-prey model, which can be given by two ordinary differential equations:

$$\frac{dX_1}{dt} = k_1 X_1 - k_2 X_1 X_2 \tag{3}$$

$$\frac{dX_2}{dt} = -k_3 X_2 + k_2 X_1 X_2 \tag{4}$$

In order to reproduce a schoolbook example two scenarios may be created by modifying two copies (clones) of `lv`:

```
R> library("simecol")
R> data(lv, package = "simecol")
R> lv1 <- lv2 <- lv
```

We now inspect default settings of initial values and parameters, modify them as required for `lv2` and simulate both scenarios:

```
R> init(lv1)
```

```
    prey predator
     0.5      1.0
```

```
R> parms(lv1)
```

```
 k1  k2  k3
0.2 0.2 0.2
```

```
R> parms(lv2)["k3"] <- 0.1
R> lv1 <- sim(lv1)
R> lv2 <- sim(lv2)
```

The outputs of `lv1` and `lv2` can be compared visually using the plotting method of the `odeModel` class (`plot(lv1)`) or with regular plotting functions after extracting the outputs (Figure 4). It is quite obvious that scenario 1 produces stable cycles and that scenario 2 is at equilibrium for the given initial values and parametrization, because of:

$$\frac{dX_1}{dt} = 0.2 \cdot 0.5 - 0.2 \cdot 0.5 \cdot 1 = 0 \tag{5}$$

$$\frac{dX_2}{dt} = -0.1 \cdot 1 + 0.2 \cdot 0.5 \cdot 1 = 0 \tag{6}$$

It is a particular advantage of R, that the complete set of statistical functions is immediately available, e.g. to inspect summary statistics like the range:

```
R> sapply(o1[c("predator", "prey")], range)
```

```
      predator      prey
[1,] 0.5001358 0.500000
[2,] 1.7563205 1.755704
```

```
R> sapply(o2[c("predator", "prey")], range)
```
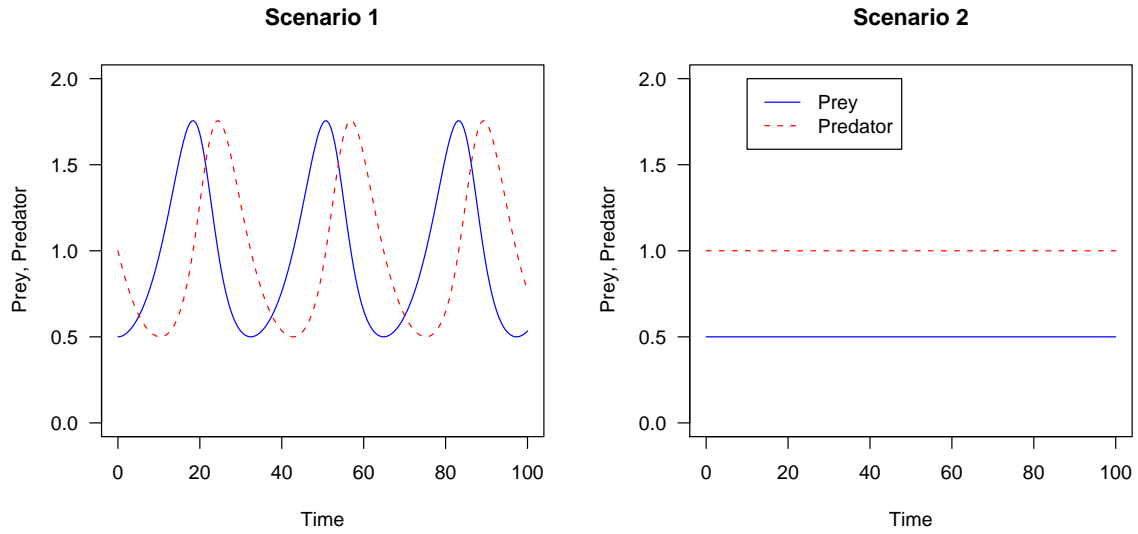
Figure 4: Two scenarios of a basic Lotka-Volterra model. Scenario 1 (left) shows stable cycles, Scenario 2 (right) is at equilibrium.

```
      predator prey
[1,]         1  0.5
[2,]         1  0.5
```

The identity of the lower and upper limits for scenario 2 confirm the equilibrium state. Moreover, the period length of the cycles of scenario 1 can be analysed by means of spectral analysis:

```
R> tlv <- times(lv1)
R> ots <- ts(o1[c("predator", "prey")], start = tlv["from"],
+      end = tlv["to"], deltat = tlv["by"])
R> sp <- spectrum(ots, spans = c(3, 3), log = "no")
R> 1/sp$freq[sp$spec[, 1] == max(sp$spec[, 1])]
```

```
[1] 36
```

which yields an estimated period length of approximately 36 time units.

5. Implementation of simecol models

5.1. Lotka-Volterra model

The implementation of the Lotka-Volterra equations is straightforward and results in a compact S4 object (Table 1). The two equations (Eq. 3, 4) can easily be put into the main function and there is no need for sub-equations. The code can be made even simpler without

Table 1: Implementation example of the elementary Lotka-Volterra model

```
lv <- new("odeModel",
  main = function (time, init, parms, ...) {
    x <- init
    p <- parms
    dx1 <-   p["k1"] * x[1] - p["k2"] * x[1] * x[2]
    dx2 <- - p["k3"] * x[2] + p["k2"] * x[1] * x[2]
    list(c(dx1, dx2))
  },
  parms  = c(k1=0.2, k2=0.2, k3=0.2),
  times  = c(from=0, to=100, by=0.5),
  init   = c(prey=0.5, predator=1),
  solver = "rk4"
)
```

the two assignments at the beginning of main, but with respect to more structured models we found it generally advantageous to keep the default values of the names in the parameter line and on the other hand to use common symbols in the equations.

5.2. Models with nested subequations

For large models with numerous equations or for models with alternative (i.e. exchangeable) submodels it may be preferable to use a separate structure. Although **simecol** principally allows implementing subroutines as local functions of the `main` slot or even directly in the user workspace such a strategy would not be in line with our design goals. Instead, the `equation`-slot of the `simObj` class definition provides the structure where relevant submodels and model equations are stored. Consequent usage of the `equation` slot helps to increase the readability of the `main` function, leads to more structurized code and complies with the object-oriented paradigm. Moreover, the `equation` slot can be used to store alternative submodels, see Table 2 for a small example.

In this example, two versions of the functional response can be enabled alternatively by assigning one of `f1` or `f2` to `f` via `equations` (last line of the Table 2) and with the same mechanism it is possible to introduce further functional response curves.

The example shows also several techniques for scoping: (i) the parameter vector is "unpacked" using `with`[7], (ii) parameters are explicitly passed to subequations and (iii) slot functions of `equations` can be used without explicit pass through, a functionality that is provided by the `solver` functions. The result is, that all elements of the `equations` slot are visible within `main` and within all other functions of `equations`.

---

[7]This requires conversion of the parameter vector into a list. Parameter vectors are only used in the `odeModel` class to ease implementation of teaching models, all other classes natively use lists.

Table 2: Uniform Period Chaotic Amplitude Model after Blasius *et al.* (1999). Note that function `f1` is nested within `f2`.

```
upca <- new("odeModel",
  main = function(time, init, parms) {
    u       <- init[1]
    v       <- init[2]
    w       <- init[3]
    with(as.list(parms), {
      du <-  a * u           - alpha1 * f(u, v, k1)
      dv <- -b * v           + alpha1 * f(u, v, k1) - alpha2 * f(v, w, k2)
      dw <- -c * (w - wstar) + alpha2 * f(v, w, k2)
      list(c(du, dv, dw))
   })
  },
  equations  = list(
    f1 = function(x, y, k){x * y},                     # Lotka-Volterra
    f2 = function(x, y, k){f1(x, y, k) / (1 + k * x)} # Holling II
  ),
  times  = c(from=0, to=100, by=0.1),
  parms  = c(a=1, b=1, c=10, alpha1=0.2, alpha2=1,
             k1=0.05, k2=0, wstar=0.006),
  init = c(u=10, v=5, w=0.1),
  solver = "lsoda"
)

equations(upca)$f <- equations(upca)$f1
```

5.3. Input data

The simulation models presented so far are autonomous, i.e. they have no external forcing data (matrix **u** in Figure 1). Such time dependent data, e.g. food availability or meteorological conditions, which are required in many practical cases can be provided in the `inputs` slot. In order to give a minimal example we may create a new `odeModel` by modifying a clone `lv_ef` of the elementary predator-prey model. To enable external forcing a modified version of the `main` slot is introduced, that simulates substrate (S) dependent growth of the prey population:

```
R> lv_ef <- lv
R> main(lv_ef) <- function(time, init, parms, ...) {
+      x <- init
+      p <- parms
+      S <- approxTime1(inputs, time, rule = 2)["s.in"]
+      dx1 <- S * p["k1"] * x[1] - p["k2"] * x[1] * x[2]
```
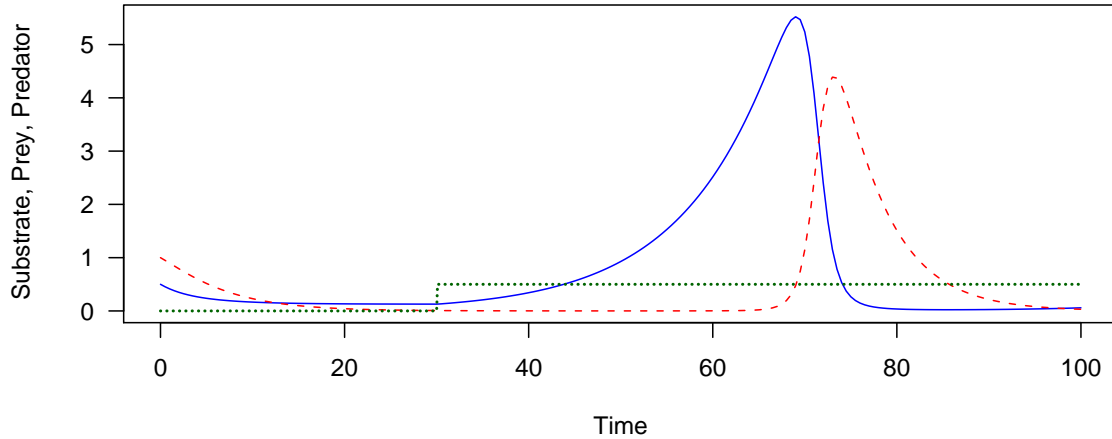
Figure 5: Externally forced predator-prey model (prey: blue, solid; predator: red, dashed) with resource (green dotted line).

```
+        dx2 <- -p["k3"] * x[2] + p["k2"] * x[1] * x[2]
+        list(c(dx1, dx2))
+   }
```

For linear interpolation the utility function `approxTime1` is used here to read the input at correct time steps from the input matrix, which can be given as:

```
R> inputs(lv_ef) <- as.matrix(data.frame(time = c(0, 30, 30.1,
+        100), s.in = c(0, 0, 0.5, 0.5)))
```

Note, that inputs are converted into a matrix for performance reasons because otherwise repeated conversions were performed by `approxTime1`, or similarly by `approx`, which would be time consuming, especially for larger input data sets.

The resulting model can then be easily simulated and plotted and results in Figure 5:

```
R> o <- out(sim(lv_ef))
R> matplot(o$time, o[2:3], xlab = "Time", ylab = "Substrate, Prey, Predator",
+        type = "l", lty = c("solid", "dashed"), col = c("blue",
+            "red"), las = 1)
R> inp <- as.data.frame(inputs(lv_ef))
R> lines(inp$time, inp$s.in, col = "darkgreen", lwd = 2, lty = "11")
```

5.4. Initializing

Sometimes, it may be required to perform computations while initializing a `simObj`. This may be either required to ensure consistency between different slots (e.g. parameters, inputs and

Table 3: Predator-prey simulation with stochastic input variables. The example is derived from the externally forced object `lv_ef`. An initialisation function `initfunc` is provided which is called by `initialize` and returns a re-initialized `obj` with a new random sample of input values. The utility function `fromtoby` is used to expand the time vector from its compact form `c(from=, to=, by=)` into a sequence.

```
lv_efr <- lv_ef
tt <- fromtoby(times(lv_efr))
o <- matrix(0, nrow = length(tt), ncol = 10)
initfunc(lv_efr) <- function(obj) {
    tt <- fromtoby(times(obj))
    inputs(obj) <- as.matrix(data.frame(time = tt, s.in = pmax(rnorm(tt,
        mean = 1, sd = 0.5), 0)))
    obj
}
for (i in 1:10) {
    lv_efr <- initialize(lv_efr)
    lv_efr <- sim(lv_efr)
    o[, i] <- out(lv_efr)$prey
}
matplot(tt, o, xlab = "Time", ylab = "Prey", las = 1, type = "l")
```
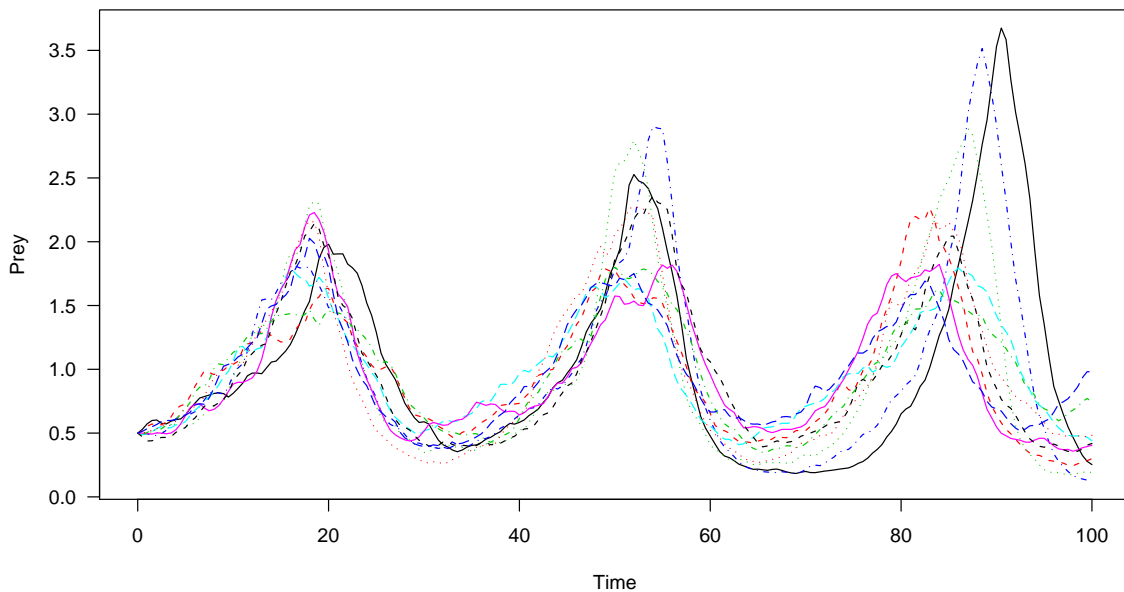

Figure 6: Ten stochastic realizations of the model from Table 3.

initial values) to perform error checking or to create non-deterministic variants. Initializing methods, which exist in R as class methods of the generic `initialize`, are called either explicitly or implicitly during object creation. The syntax allows, in principal, two different modes of use. One can either provide all slots of the object in creation as named arguments to `new` or one can provide an existing `simObj` as the first un-named argument to `initialize` in order to get a re-initialized clone.[8]

In the case of `simObj` this mechanism is extended by an optionally existing function slot `initfunc`, which is executed during the object creation process. Object creation is then as follows: in the first step an incomplete object is created internally via `new` according to the slots given and in the second step this object in creation is passed to the `obj` argument of `initfunc` which performs the final steps and returns the complete object.

It would, of course, also be possible to create a provisional object first and to modify it afterwards with accessor functions, but `initfunc` provides a more efficient solution and helps to ensure consistency, e.g. between parameters and inputs, between `times` and `inputs` or between different state variables.

In the example shown in Table 3 new instances with different stochastic realizations of the input variables are created and simulated (see Figure 6). Note that `initfunc` is called automatically every time, when new instances are created via `new` or `initialize`.

6. Creating own models

6.1. The modeling cycle

The modeling process is an iterative cycle of tasks (see Grimm and Railsback 2005). It begins with the formulation of (i) questions and (ii) hypotheses, (iii) the translation of these questions into a specific model structure, (iv) the implementation of the model in form of computer software, (v) the analysis, test and (in most cases) revision of the model, and (vi) communication of the model and its results to the scientific community. Another view is given by Fowler and Scott (1997), who with respect to software modeling suggested to distiguish three different perspectives:

1. Conceptional perspective,

2. Specification perspective,

3. Implementation perspective.

These perspectives are complementary to the tasks defined by Grimm and Railsback (2005) when tasks (i)–(ii) are regarded as conceptional and task (iii) as specification. In the following we concentrate on task (iv) to explain by means of a real, but still simple example, how a specified model can be implemented using R and the **simecol** software.

6.2. Conceptional perspective: an individual-based model of Daphnia

The scientific purpose of the *Daphnia* model given here was the analysis of demographic effects of *Daphnia* (water flea) populations. Two main hypotheses should be tested:

---

[8]Initialization is now done automatically before each call to sim (introduced in version 0.6).

- Size-selective predation leads to an increased population mortality rate, compared to non-selective predation by fish (Mehner *et al.* 1998).

- In comparison to predictions from the conventional Lotka-Volterra approach the inclusion of demographic effects results in a delayed but then inexpectedly rapid decline of abundance during periods of food limitation due to ageing effects (Hülsmann and Voigt 2002).

Due to a multiple number of important features, the genus *Daphnia* (water flea) is an outstanding model organism in limnology, toxicology and population ecology, so results derived on this example may be of general interest to other areas as well.

The *Daphnia* model consists of three general parts:

1. A semi-empirical model of temperature and food dependent somatic growth and egg production derived from laboratory experiments (TeFI = temperature-food-interaction model) according to Rinke and Petzoldt (2003),

2. An empirical function of egg development time after Bottrell *et al.* (1976),

3. A non-spatial individual-based simulation of population dynamics.

Individual-based models (IMBs) are a popular technique in ecological modeling (DeAngelis and Gross 1992; Grimm 1999; Grimm and Railsback 2005). It is our aim to demonstrate how such models can be implemented with **simecol**.

6.3. Model specification

The state of the system is defined as a sample of individuals, each having four states: age, size, number of eggs and age of eggs. Population development is dependend on two environmental variables, food (phytoplankton, given in $mg\,L^{-1}$ carbon) and temperature (in °C). The model is simulated in fixed time steps (usually 0.1 day) over a period of several days up to a few months. The time scales are selected with respect to the egg development time, which is about 4.4 days at 15 °C(Bottrell *et al.* 1976).

The life cycle of *Daphnia* starts with the release of neonate individuals of a given size (L_0) from the brood chamber of the mother into the water. Somatic growth follows the von Bertalanffy growth equation (von Bertalanffy 1957), depending on several empirical parameters. As soon as an individual reaches a fixed size at maturity (SAM) a clutch of eggs is produced (spawned), whereby the clutch size (number of eggs) is controlled by food availablility. After a temperature dependend egg development time the individuals from this clutch are released (hatched) and the cycle is started again (parthenogenetic, i.e. asexual reproduction).

Mortality can be modelled with arbitrary deterministic or stochastic mortality functions, e.g. size dependent mortality due to fish predation, but for the first simulation a deterministic fixed maximum age is used. All equations and parameters are given in detail in Rinke and Petzoldt (2003) and although more elaborate bioenergetic *Daphnia* models are available in the meantime (Rinke and Vijverberg 2005; Rinke *et al.* 2005), the relatively simple model given here should be sufficient for the intended purpose.

6.4. Model implementation

Definition of a user-defined subclass

A subclass for non-spatial individual-based models is not yet available in **simecol**, but can be easily derived from `simObj` as class with appropriate data types, in particular with a `data.frame` for the table of the individuals stored in `init`:

```
R> setClass("indbasedModel", representation(parms = "list",
+      init = "data.frame"), contains = "simObj")
```

Implementation of the model equations

The implementation which is provided in Table 4 and 5 in the appendix starts with the selection of an appropriate data structure for the state variables. A table of individuals with four columns: age, size, number of eggs and age of eggs (`eggage`) is realized as data frame with one row for each individual. The data frame is initialized with an arbitrary number of start individuals (e.g. one single juvenile animal in the `init` slot).

The `main` function simulates the life cycle of *Daphnia* and calls the sub-equations `live`, `survive` and `hatch` which implement the following processes:

live: The age of all individuals and the egg-age for individuals with eggs is incremented by the actual time step `DELTAT`. Then, the empirical function `tefi` is called to estimate length and potential number of eggs as a function of age, food and temperature. The data frame of individuals is then updated and for all adult individuals (size > size at maturity, SAM) which actually have no eggs the appropriate number of eggs is initialized.

survive: The survival function returns the subset of surviving individuals. Note that it is particularly easy in R to implement survival with the `subset` function by simply applying a logical rule to the table of individuals and returning only those rows which match the condition.

hatch: In a first step the the actual egg age is compared with the egg development time. Then the total number of mature eggs is counted and a data frame (`newinds`) with an appropriate number of individuals is created (function `newdaphnia`. Population growth occurs by appending the data frame with newborns (`newinds`) to the data frame of the surviving (`inds`).

All functions of the life cycle receive the actual table of individuals (`init`) as their first argument and return an updated table `inds` which is then passed back to `init`.

The model is simulated by iteration over the time vector. Note that in contrast to ODE models the `main` function explicitly returns the new state and not derivatives. To account for this, the `iteration` algorithm is to be used here and not one of the ODE solvers like `euler`, `rk4` or `lsoda`.

A number of constant parameters is needed by the empirical model (see Rinke and Petzoldt 2003, for details), which are represented as list within the `parms` slot.

6.5. Model simulation

With the `ibm_Daphnia` object derived from the `indbasedModel` class and given as complete source code in Tables 4 and 5 it is now possible to perform a first simulation:

```
R> solver(ibm_daphnia) <- "iteration"
R> ibm_daphnia <- sim(ibm_daphnia)
```

This already works with the `iteration` method provided by the package, but the default behavior may not be optimal for the concrete subclass.

One disadvantage here is the fact that the default `iteration` algorithm stores the complete state data structure (i.e. the complete data frame) for each time step as list in the `out` slot. This behavior is rather memory consuming for individual-based simulations with several hundred or thousand individuals. Moreover, no adequate plotting method is currently available for such a list of data frames and therefore the default `plot(simObj)` method simply returns a warning message.

6.6. Class-specific functions and methods

Depending on the complexity of the model it may be necessary to supply either an own solver function or a complete `sim` method. The difference is that only one `sim` method is available for one particular class, but several solver functions may be provided as alternatives for one class, either as `S4` methods with different names or as ordinary (non generic) functions.

In most cases it should be sufficient to write class specific solvers, but for complicated data structures or hybrid model architectures it may be necessary to provide class specific `sim` methods. In case of the individual-based *Daphnia* model, the solver should be of type "iterator" but with additional functionality to reduce the amount of data stored in `out`. To do this, `mysolver` given in Table 6 has a local function `observer`, which for each time step returns one line of summary statistics for all individuals. Additionally, it would be also possible to write data to logfiles, to print selected data to screen or to display animated graphics during simulation.

The argument naming of the solver functions is compatible with the ODE solvers of the **odesolve**-package with respect to the first four arguments. Moreover, some essential functionality must be provided by all solvers:

1. Extraction of slots of the `simObj` (argument `y`) to local variables, expansion of `y@times` via `fromtoby`, `attach` and `detach` for the list of equations as given in the example,

2. Iteration loop or any other appropriate numeric algorithm,

3. Assignment of the special parameter DELTAT (optional, if needed by the model),

4. Accumulation of essential simulation results to the outputs (`out`-slot) and assignment of explanatory variable names, in this case done by `observer`.

Depending on the data structure, it is also possible to write a class specific plot function:

```
R> setMethod("plot", c("indbasedModel", "missing"), function(x,
+      y, ...) {
+      o <- out(x)
+      par(mfrow = c(2, 2))
+      plot(o$times, o$meanage, type = "l", xlab = "Time",
+          ylab = "Mean age (d)")
+      plot(o$times, o$meaneggs, type = "l", xlab = "Time",
+          ylab = "Eggs per individual")
+      plot(o$times, o$number, type = "l", xlab = "Time",
+          ylab = "Abundance")
+      plot(o$times, o$number, type = "l", xlab = "Time",
+          ylab = "Abundance", log = "y")
+ })
```

6.7. Model application

Now, the model can be simulated and used for the intended application, e.g. hypothesis testing, parameter estimation or scenario analysis:

```
R> solver(ibm_daphnia) <- "myiteration"
R> ibm_daphnia <- sim(ibm_daphnia)
R> plot(ibm_daphnia)
```

It is beyond the scope of this paper to provide an overview over simulation techniques or to answer domain specific questions about *Daphnia* population dynamics; however, the following example is intended to give an impression how **simecol** models can be used in practice. The example deals with the effect of size-selective predation, similar to the more extensive analysis of Mooij *et al.* (1997). Four scenarios will be compared:

Sc0: no mortality at all,

Sc1: constant mortality (independent of body length),

Sc2: small individuals preferred (typical for invertebrate predators like *Chaoborus*, phantom midge larvae),

Sc3: large individuals preferred (typical for adult fish).

At the first step we create one clone of the `daphnia_ibm`-object, assign settings common to all scenarios and an initial sample population:

```
R> Sc0 <- ibm_daphnia
R> times(Sc0) <- c(from = 0, to = 30, by = 0.2)
R> parms(Sc0)[c("temp", "food", "mort")] <- c(15, 0.4, 0.1)
R> init(Sc0) <- data.frame(age = rep(10, 50), size = rep(2.5,
+      50), eggs = rep(5, 50), eggage = runif(50, 0, 4))
```
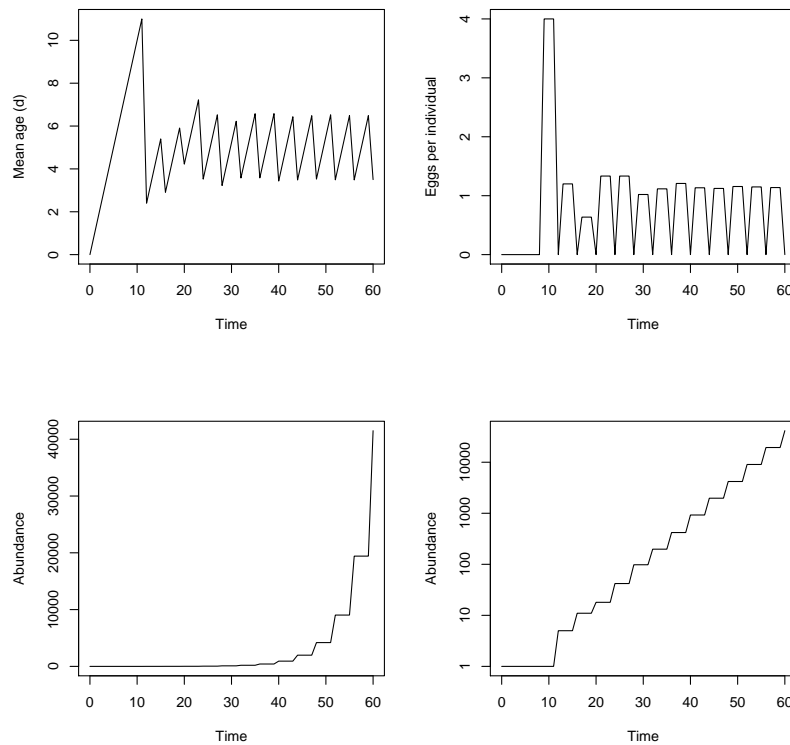
Figure 7: Result of the `plot` method of the *Daphnia* model, top: mean age of the population and number of eggs indicating synchronized population development; bottom: exponential population growth in linear resp. logarithmic scale.

Then we replace the default `survive`-function with a more general one which depends on a user-specified mortality function `fmort`:

```
R> equations(Sc0)$survive = function(inds, parms) {
+     abundance <- nrow(inds)
+     rnd <- runif(abundance)
+     mort <- fmort(parms$mort, inds$size) * parms$DELTAT
+     subset(inds, rnd > mort)
+ }
```

Copies of object `Sc0` are created and modified according to the scenario specification. In the example below we have two functions with constant mortality and two other functions where per capita mortality is higher for the larger or smaller individuals, respectively:

```
R> Sc1 <- Sc2 <- Sc3 <- Sc0
R> equations(Sc0)$fmort <- function(mort, x) 0
R> equations(Sc1)$fmort <- function(mort, x) mort
R> equations(Sc2)$fmort <- function(mort, x) {
+     mort * 2 * rank(-x)/(length(x) + 1)
```
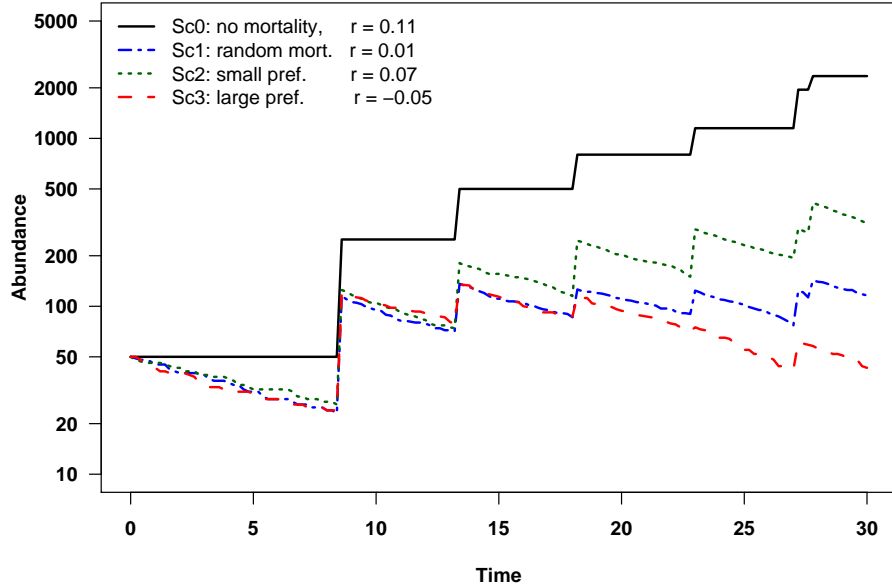
Figure 8: Time series of *Daphnia* abundance for different scenarios with non-selective resp. size selective mortality. Population growth rates (r in d^{-1}) were approximated by log-linear regression for all data points after an initial period of 10 days.

```
+ }
R> equations(Sc3)$fmort <- function(mort, x) {
+     mort * 2 * rank(x)/(length(x) + 1)
+ }
```

Finally, the scenarios can be simulated, either line by line as in Section 4.2 or listwise with `lapply`:

```
sc <- lapply(list(Sc0=Sc0, Sc1=Sc1, Sc2=Sc2, Sc3=Sc3), sim)
```

The result shows very clearly the influence of demography on population growth (Figure 8). Given that the population growth rate r without any mortality (i.e. equal to the birth rate b) is approximately 0.11d^{-1} in `Sc0` and the mortality rate d is set to 0.1d^{-1}, it is plausible that the population growth rate in `Sc1` is:

$$r = b - d \approx 0.01\mathrm{d}^{-1}$$

In case of size-selective predation, demography has to be taken into account in order to get realistic estimations of r. The simulation shows an increased population loss in case of fish predation (`Sc3`, $r = -0.05$) and a lower effect in case of *Chaoborus* (`Sc2`, $r = 0.07$). Please see Mooij *et al.* (1997, 2003) for details and how the results may depend on fecundity of the prey, the shape of the selection function and the dynamics of predator and prey.

7. Discussion

The main contribution of the **simecol** package is the proposal of a generalized, declarative structure to describe ecological models. This structure was inspired by the state space representation used in control theory and is intended as a pragmatic solution to unify the upcoming diversity of R implementations of ecological models. The object-oriented `simObj` structure may be useful also in other areas and for other models like continuous-time Markov processes and stochastic differential equations.

With the set of examples presented and some additional models developed in our workgroup, the matrix-oriented R language was found to be well suited for model development (rapid prototyping) and model evaluation. According to our experience, a structured OOP style is more efficient compared to a purely functional style, or even worse, ad-hoc programming.

The functional OOP system of R is different from languages like JAVA or C++ and the approach of generic functions for common tasks seems to be more appropriate for statistical data analysis than for ecological simulation models which have not only variable data but also variable code. Moreover, the lack of references and the invisibility of member variables in slot functions of the same object was seemingly inconvenient and needed re-thinking. However, the R language with its Scheme heritage (Ihaka and Gentleman 1996) is a "programmable programming language". Lexical scoping and local environments (Gentleman and Ihaka 2000) allow to change its default behavior if needed. There were temptations to apply an alternative OOP paradigm that allows for references e.g. **R.oo** (Bengtsson 2003) or **proto** (Kates and Petzoldt 2005), but it was decided to stay with the default behavior as much as possible. Similarly, we used only flat object hierarchies and abandoned delegation-based approaches and instead suggest cloning (creation time sharing) as a standard technique to create derived objects.

At a first look R seems to be less suited for large applications, e.g. turbulence models, where C and FORTRAN are standard or for complex individual-based simulations with large numbers of interacting individuals, where class-based OOP in the flavor of C++ or JAVA is regarded as more natural (Grimm and Railsback 2005). However, even such applications can take advantage of **simecol**, either because of vectorization in R (`subset` is in fact highly efficient) or due to the possibility to embed compiled code as shared library. For large applications or external simulation programs, **simecol** objects can be constructed as an interface provided that the external program is open enough to be linked or at least is callable in batch mode.

The package is designed to be open for local extensions and further evolution of the package itself. A limited number of classes will follow, e.g. for individual-based models similar to the *Daphnia* example or for purely statistical models like neural networks. An integrated parameter estimation functionality may follow as well as an interface to quantitative and qualitative model evaluation criteria (Jachner *et al.* this volume). Moreover, interfaces to other promising approaches to solve simulation models in R may be worth to be established, e.g. to the XML based description language of the bioconductor package **SBMLR** (Radivoyevitch 2004), or to the nonlinear mixed effects modelling package **nlmeODE** of Tornø *et al.* (2004) who independently developed a similar list-based object structure for a class of ordinary differential equation models.

Another appealing approach is the stoichiometry-matrix based approach for ODE models of aquatic systems (wastewater treatment, biofilm, rivers and lakes, `http://www.eawag.ch/organisation/abteilungen/siam/lehre/Modaqecosys/`). These R scripts, developed by a

prominent group in water modeling (e.g. Reichert 1994; Reichert *et al.* 2001), are currently used for teaching of aquatic modeling together with model assessment like sensitivity and uncertainty analysis, optimization, and frequentist or Bayesian model tests.

Our work presented so far can serve as a starting point and demonstrates, that R together with OOP is well suited as a medium for the development, distribution and share of ecological modeling code. Reference applications and utility functions will help ecologists to structure their work. The open source license of R and its accompanying packages should encourage own applications, which remain under complete control of the developer. Moreover, the intentionally lightweight character of **simecol** and the compact code of the solutions would enable the user to unhinge his model from **simecol** whenever required and to port it to other systems. As a conclusion, one can make nothing wrong when starting to model with R but it may be possible that one stays with it for a long time.

Acknowledgments

References

Bengtsson H (2003). "The **R.oo** Package – Object-Oriented Programming with References Using Standard R Code." In K Hornik, F Leisch, A Zeileis (eds.), "Proceedings of the 3rd International Workshop on Distributed Statistical Computing (DSC 2003)," pp. 1–18. Vienna, Austria. ISSN 1609-395X, URL http://www.maths.lth.se/help/R/R.oo/.

Benz J, Hoch R, Legovic T (2001). "ECOBAS - Modelling and Documentation." *Ecological Modelling*, **138**, 3–15.

Blasius B, Huppert A, Stone L (1999). "Complex Dynamics and Phase Synchronization in Spatially Extended Ecological Systems." *Nature*, **399**, 354–359.

Bossel H (1992). "Real-structure Process Description as the Basis of Understanding Ecosystems and Their Development." *Ecological Modelling*, **63**(1-4), 261–276.

Bottrell HH, Duncan A, Gliwicz ZM, Grygierek E, Herzig A, Hillbricht-Ilkowska A, Kurasawa H, Larsson P, Weglenska T (1976). "A Review of Some Problems in Zooplankton Production Studies." *Norwegian Journal of Zoology*, **24**, 419–456.

Chambers JM (2000). "Users, Programmers, and Statistical Software." *Journal of Computational and Graphical Statistics*, **9**(3), 404–422.

Chambers JM (2001). "Classes and Methods in the S Language." URL http://www.omegahat.org/RSMethods/Intro.pdf.

Cribari-Neto F, Zarkos SG (1999). "R: Yet Another Econometric Programming Environment." *Journal of Applied Econometrics*, **14**(3), 319–329.

DeAngelis DL, Gross LJ (eds.) (1992). *Individual-Based Models and Approaches in Ecology: Populations, Communities, and Ecosystems.* Chapmann and Hall, Knoxwille, Tennessee. Proceedings of a Symposium/Workshop.

Dunning JBJ, Stewart DJ, Danielson BJ, Noon BR, Root TL, Lamberson RH, Stevens EE (1995). "Spatially Explicit Population Models: Current Forms and Uses." *Ecological Applications*, **5**, 3–11.

Fowler M, Scott K (1997). *UML Distilled. Applying the Standard Object Modelling Language.* Addison Wesley.

Fussmann GF, Ellner SP, Hairston NGJ (2003). "Evolution as a Critical Component of Plankton Dynamics." *Proceedings of the Royal Society of London Series B*, **270**, 1015–1022.

Gentleman R, Ihaka R (2000). "Lexical Scope and Statistical Computing." *Journal of Computational and Graphical Statistics*, **9**(3), 491–508.

Grimm V (1999). "Ten Years of Individual-Based Modelling in Ecology: What Have We Learned and What Could We Learn in Future?" *Ecological Modelling*, **115**, 129–148.

Grimm V, Berger U, Bastiansen F, Eliassen S, Ginot V, Giske J, Goss-Custard J, Grand T, Heinz SK, Huse G, Huth A, Jepsen JU, Jørgensen C, Mooij WM, Müller B, Péer G, Piou C, Railsback SF, Robbins AM, Robbins MM, Rossmanith E, Rüger N, Strand E, Souissi S, Stillman RA, Vabø R, Visser U, DeAngelis DL (2006). "A Standard Protocol for Describing Individual-Based and Agent-Based Models." *Ecological Modelling*, **198**, 115–126.

Grimm V, Railsback SF (2005). *Individual-based Modeling and Ecology.* Princeton University Press, Princeton N.J.

Gurney WSC, Nisbet RM (1998). *Ecological Dynamics.* Oxford University Press, New York, Oxford.

Hartley DM, Jr MJG, Smith DL (2006). "Hyperinfectivity: A Critical Element in the Ability of *V. cholerae* to Cause Epidemics?" *PLoS Medicine*, **3**(1), 63–69. doi:10.1371/journal.pmed.0030007.

Hülsmann S, Voigt H (2002). "Life History of *Daphnia galeata* in a Hypertrophic Reservoir and Consequences of Non-consumptive Mortality for the Initiation of a Midsummer Decline." *Freshwater Biology*, **47**, 2313–2324.

Ihaka R, Gentleman R (1996). "R: A Language for Data Analysis and Graphics." *Journal of Computational and Graphical Statistics*, **5**(3), 299–314.

Jachner S, van den Boogaart G, Petzoldt T (this volume). "Statistical Methods for the Qualitative Assessment of Dynamic Models with Time Delay (R Package **qualV**)." *Journal of Statistical Software.*

Jensen MA, Faruque SM, Mekalanos JJ, Levin BR (2006). "Modeling the Role of Bacteriophage in the Control of Cholera Outbreaks." *PNAS*, **103**, 4652–4657.

Kates L, Petzoldt T (2005). *The R* **proto** *Package.* Package vignette of the CRAN **proto** package, URL http://cran.r-project.org/doc/vignettes/proto/proto.pdf.

Levey DJ, Bolker BM, Tewksbury JJ, Sargent S, Haddad NM (2005). "Effects of Landscape Corridors on Seed Dispersal by Birds." *Science*, **309**, 146–148.

Ludyk G (1995). *Theoretische Regelungstechnik 1: Grundlagen, Synthese linearer Regelungssysteme.* Springer, Berlin.

Mehner T, Hülsmann S, Worischka S, Plewa M, Benndorf J (1998). "Is the Midsummer Decline of *Daphnia* Really Induced by Age-0 Fish Predation? Comparison of Fish Consumption and *Daphnia* Mortality and Life History Parameters in a Biomanipulated Reservoir." *Journal of Plankton Research*, **20**, 1797–1811.

Mooij WM, Boersma M (1996). "An Object Oriented Simulation Framework for Individual-Based Simulations (OSIRIS): *Daphnia* Population Dynamics as an Example." *Ecological Modelling*, **93**, 139–153.

Mooij WM, Boersma M, Vijverberg J (1997). "The effect of size-selective predation on the population growth rate, the production to biomass ratio and the population structure of Daphnia galeata: a modelling approach." *Archiv für Hydrobiologie Special Issue Advances in Limnology*, **49**, 87–97.

Mooij WM, Hülsmann S, Vijverberg J, Veen A, Lammens EHRR (2003). "Modeling *Daphnia* Population Dynamics and Demography Under Natural Conditions." *Hydrobiologia*, **491**, 19–34.

Mächler M (2004). "Good Programming Practice." Keynote lecture at the useR!-2004 conference, URL http://www.ci.tuwien.ac.at/Conferences/useR-2004/Keynotes/Maechler.pdf.

Petzoldt T (2003). "R as a Simulation Platform in Ecological Modelling." *R News*, **3**(3), 8–16.

Petzoldt T, Rinke K (2007). "**simecol**: An Object-Oriented Framework for Ecological Modeling in R." *Journal of Statistical Software*, **22**(9), 1–31. ISSN 1548-7660. URL http://www.jstatsoft.org/v22/i09.

Radivoyevitch T (2004). "A Two-Way Interface between Limited Systems Biology Markup Language and R." *BMC Bioinformatics*, **5**.

R Development Core Team (2006). *R: A Language and Environment for Statistical Computing.* R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL http://www.R-project.org.

Reichert P (1994). "AQUASIM - A Tool for Simulation and Data Analysis of Aquatic Systems." *Water Science and Technology*, **30**(2), 21–30.

Reichert P, Borchardt D, Henze M, Rauch W, Shanahan P, Somlyódy L, Vanrolleghem P (2001). "River Water Quality Model No. 1 (RWQM1): II. Biochemical Process Equations." *Water Science and Technology*, **43**, 11–30.

Rinke K, Petzoldt T (2003). "Modelling the Effects of Temperature and Food on Individual Growth and Reproduction of *Daphnia* and Their Consequences on the Population Level." *Limnologica*, **33**(4), 293–304.

Rinke K, Vijverberg J (2005). "A Model Approach to Evaluate the Effect of Temperature and Food Concentration an Individual Life-History and Population Dynamics of *Daphnia*." *Ecological Modelling*, **186**, 326–344.

Rinke K, Vijverberg J, Petzoldt T, Benndorf J (2005). "Individual and Population Level Dynamics of *Daphnia* at Varying Conditions of Food, Temperature and Fish Predation: A Model Approach." *Verhandlungen der Internationalen Vereinigung für Limnologie*, **29**, 310–314.

Rolinski S, Petzoldt T, Baumert HZ, Bigalke K, Horn H, Benndorf J (2005). "Das physikalisch-ökologisch gekoppelte Talsperrenmodell." *Wasserwirtschaft*, **95**, 34–38.

Tornø CW, Agersø H, Jonsson EN, Madsen H, Nielsen HA (2004). "Non-Linear Mixed-Effects Pharmacokinetic/Pharmacodynamic Modelling in NLME Using Differential Equations." *Computer Methods and Programs in Biomedicine*, **76**(1), 31–40.

van der Maas HLJ, Dolan CV, Grasman RPPP, Wicherts JM, Huizenga HM, Raijmakers MEJ (2006). "A Dynamical Model of General Intelligence: The Positive Manifold of Intelligence by Mutualism." *Psychological Review*, **113**(4), 842–861.

von Bertalanffy L (1957). "Quantitative Laws in Metabolism and Growth." *Quartely Review of Biology*, **32**, 217–231.

Wolkenhauer O, Ullah M, Wellstead P, Cho KH (2005). "The Dynamic Systems Approach to Control and Regulation of Intracellular Networks." *FEBS Letters*, **579**, 1846–1853.

Zeileis A, Leisch F, Kleiber C, Hornik K (2005). "Monitoring structural change in dynamic econometric models." *Journal of Applied Econometrics*, **20**(1), 99–121. URL http://dx.doi.org/10.1002/jae.776.

A. The individual-based Daphnia model

Table 4: Individual-based *Daphnia* model (part I, class definition, main equation, parameters, initial state, time steps, solver)

```
library("simecol")
setClass("indbasedModel",
  representation(parms  = "list", init   = "data.frame"), contains = "simObj"
)

ibm_daphnia <- new("indbasedModel",
  main = function(time, init, parms) {
    init <- live(init, parms)
    init <- survive(init, parms)
    init <- hatch(init, parms)
    init
  },
  parms = list(
    # parameters of the somatic growth equation
    a1          = 1.167,    # (mm)
    a2          = 0.573,    # (mg L^-1)
    a3          = 1.420,    # (mm)
    a4          = 2.397,    # (d),
    b1          = 1.089e-2, # (d^-1)
    b2          = 0.122,    # ((deg. C)^-1)
    # parameters of the clutch size equation
    X_max_slope = 23.83,    # (eggs)
    K_s_slope   = 0.65,     # (mg L^-1)
    beta_min    = -29.28,   # (eggs)
    u_c         = 1,        # (L mg^-1) unit conversion factor
    # parameters of the individual-based model
    L_0_Hall    = 0.35,     # (mm) SON (size of neonanates) of Hall data
    L_0         = 0.65,     # (mm) SON
    SAM         = 1.50,     # (mm) SAM (size at maturity)
    maxage      = 60,       # (d)
    # constant environmental conditions
    temp        = 20,       # (deg C)
    food        = 0.5       # (mg L^-1)
  ),
  init      = data.frame(age=0, size=0.65, eggs=0, eggage=0),
  times     = c(from=0, to=60, by=1),
  solver    = "myiteration", # or default method: "iteration"
  equations = list()
)
```

Affiliation:

Table 5: Individual-based *Daphnia* model (part II, equations and algorithms)

```
equations(ibm_daphnia) <- list(
  newdaphnia = function(SON, n) {
    if (n>0) {
      data.frame(age = rep(0, n), size = SON, eggs = 0, eggage = 0)
    } else {
      NULL
    }
  },
  bottrell = function(temp) {
    exp(3.3956 + 0.2193 * log(temp) - 0.3414 * log(temp)^2)
  },
  tefi = function(time, temp, food, parms){
    with(parms, {
      deltaL <- L_0 - L_0_Hall
      k      <- b1 * exp(b2 * temp)
      L_max  <- (a1 * food)/(a2 + food) + a3 - k * a4
      L      <- L_max - (L_max - L_0_Hall) * exp (-k * time) + deltaL
      E      <- (X_max_slope * food)/(K_s_slope + food) * L +
                  beta_min * (1 - exp(-u_c * food))
      as.data.frame(cbind(L, E))
  })},
  live = function(inds, parms){
    with(parms,{
      ninds      <- nrow(inds)
      inds$age   <- inds$age + DELTAT
      inds$eggage <- ifelse(inds$size > SAM & inds$eggs > 0,
                          inds$eggage + DELTAT, 0)
      tefi_out   <- tefi(inds$age, temp, food, parms)
      inds$size  <- tefi_out$L
      neweggs    <- round(tefi_out$E)
      inds$eggs  <- ifelse(inds$size > SAM & inds$eggage==0,
                          neweggs, inds$eggs)
      inds
  })},
  survive  = function(inds, parms) subset(inds, inds$age < parms$maxage),
  hatch = function(inds, parms) {
    newinds <- NULL
    with(parms, {
      edt       <- bottrell(temp)
      have.neo  <- which(inds$eggs > 0 & inds$eggage > edt)
      eggs      <- inds$eggs[have.neo]
      new.neo   <- sum(eggs)
      inds$eggs[have.neo]  <-  inds$eggage[have.neo] <- 0
      newinds <- newdaphnia(L_0, new.neo)
      rbind(inds, newinds)
    })
  }
)
```

Table 6: Solver function and `plot` method for the *Daphnia* model

```
## a more appropriate solver (note the observer function
myiteration <- function(y, times=NULL, func=NULL, parms=NULL,
                        animate=FALSE, ...) {
  observer <- function(res) {
    # eggs, size, age, eggage
    number   <- nrow(res)
    meansize <- mean(res$size)
    meanage  <- mean(res$age)
    meaneggs <- mean(res$eggs)
    c(number=number, meansize=meansize, meanage=meanage, meaneggs=meaneggs)
  }
  init             <- y@init
  times            <- fromtoby(y@times)
  func             <- y@main
  parms            <- y@parms
  inputs           <- y@inputs
  equations        <- y@equations
  equations        <- addtoenv(equations)
  environment(func) <- environment()
  parms$DELTAT <- 0
  res <- observer(init)
  out <- res
  for (i in 2:length(times)) {
    time <- times[i]
    parms$DELTAT <- times[i] - times[i-1]
    init <- func(time, init, parms)
    res  <- observer(init)
    out  <- rbind(out, res)
   }
  row.names(out) <- NULL
  out <- cbind(times, out)
  as.data.frame(out)
}
## a plotting function that matches the output structure of the observer
setMethod("plot", c("indbasedModel", "missing"), function(x, y, ...) {
  o <- out(x)
  par(mfrow=c(2, 2))
  plot(o$times, o$meanage,  type="l", xlab="Time", ylab="Mean age (d)")
  plot(o$times, o$meaneggs, type="l", xlab="Time", ylab="Eggs per indiv.")
  plot(o$times, o$number,   type="l", xlab="Time", ylab="Abundance")
  plot(o$times, o$number, type="l", xlab="Time", ylab="Abundance", log="y")
})
## RUN the MODEL ##
ibm_daphnia <- sim(ibm_daphnia)
plot(ibm_daphnia)
```

Thomas Petzoldt
Institut für Hydrobiologie
Technische Universität Dresden
01062 Dresden, Germany
E-mail: thomas.petzoldt@tu-dresden.de
URL: http://tu-dresden.de/Members/thomas.petzoldt/

Karsten Rinke
Limnologisches Institut
Universität Konstanz
Mainaustrasse 252
Konstanz, Germany
E-mail: karsten.rinke@uni-konstanz.de
URL: http://www.uni-konstanz.de/limnologie/ags/Karsten/