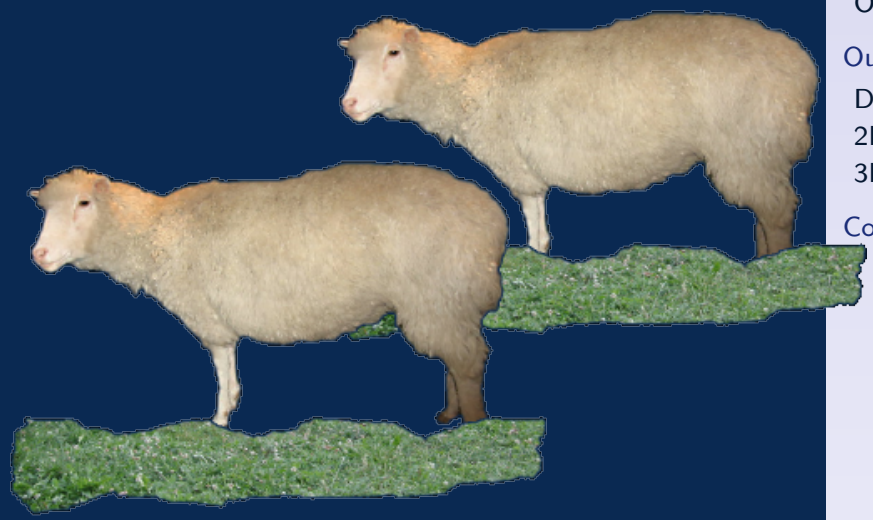
TECHNISCHE UNIVERSITÄT DRESDEN

Objects, Clones and Collections

Dynamic (Ecological) Models and Scenarios with simecol

Thomas Petzoldt

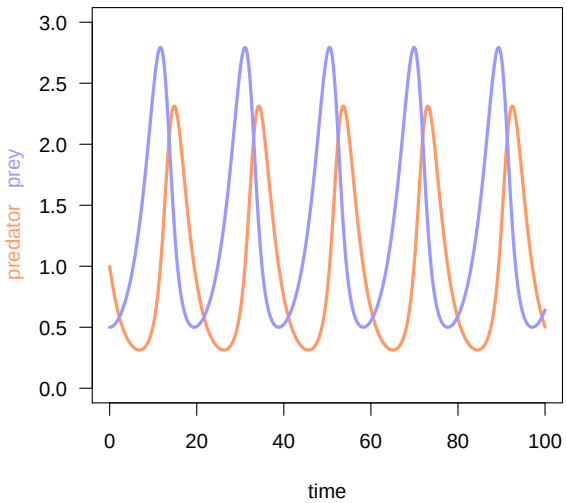


What are Ecological Models?

Two Examples from UseR!2006

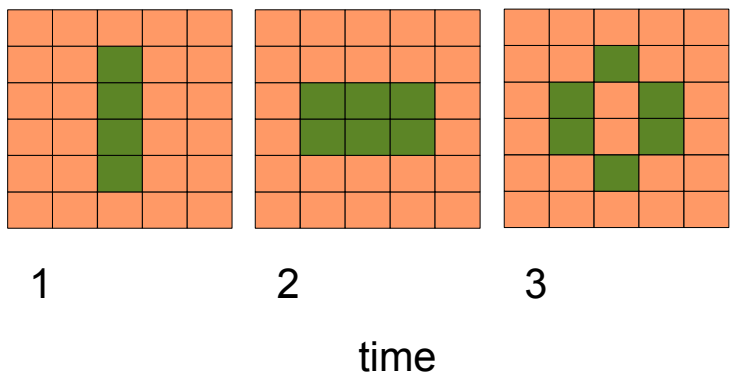
Differential Equations (e.g. Lotka-Volterra)

$$\frac{dX_1}{dt} = b \cdot X_1 - e \cdot X_1 \cdot X_2$$
$$\frac{dX_2}{dt} = d \cdot X_1 + e \cdot X_1 \cdot X_2$$



Individual-Based (Cellular automata, Random walk, . . .)

```
X = state.of(cell)
N = neighbours(cell)
if X = 1 and N in {2,3} then X := 1
  else if X = 0 and N = 3 then X := 1
    else X=0
```



Why Ecological Models in R?

R is more productive than other environments

1. More flexible than mouse-click environments,
2. Matrix orientation, Packages, Graphics, Sweave ...
3. More interactive than C++,
4. Modern computers are fast enough.

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R's Soft Skills

- Scientific development model (books and publications),
- GPL makes sharing code easy,
- Enthusiastic useR! community.

Ecological Models in R?

Problems:

- 3 Modellers – 7 Programming styles,
- Copy & Paste to derive variants and scenarios?
- Reading code? $\Rightarrow$ Better write a new program.

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Approach:

- Provide a standard approach,
- Use Object Oriented Programing – OOP,
- Package simecol: a model of ecological models.

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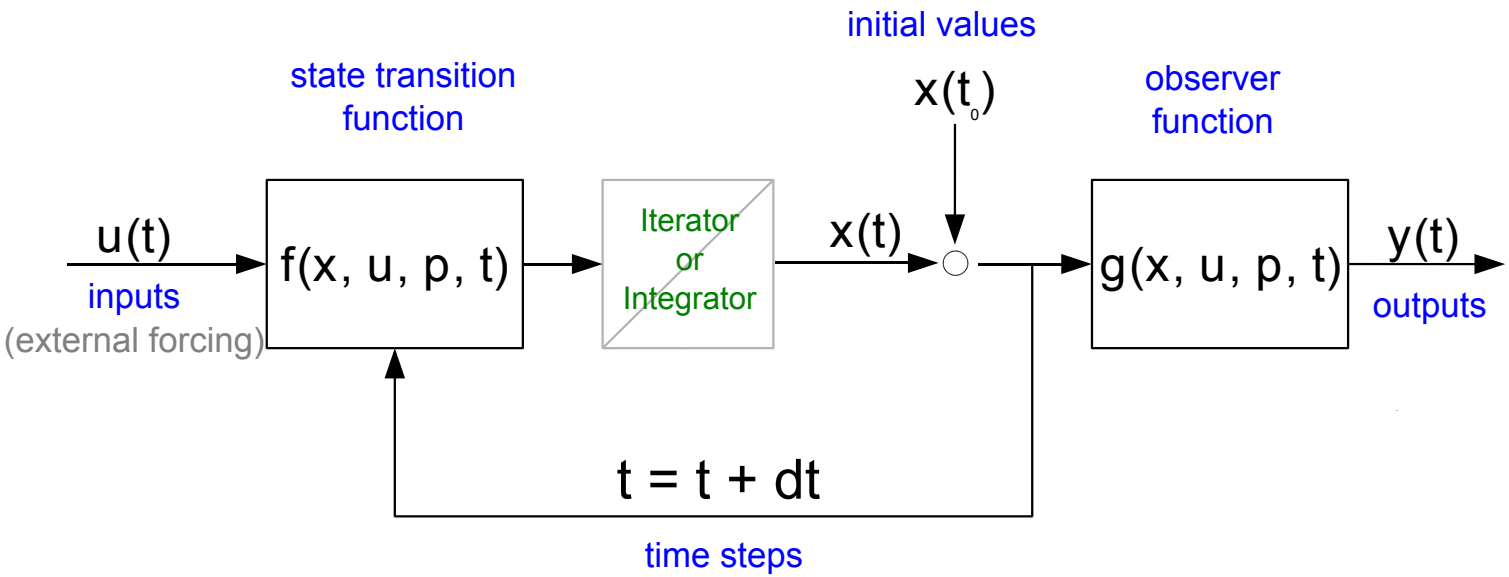
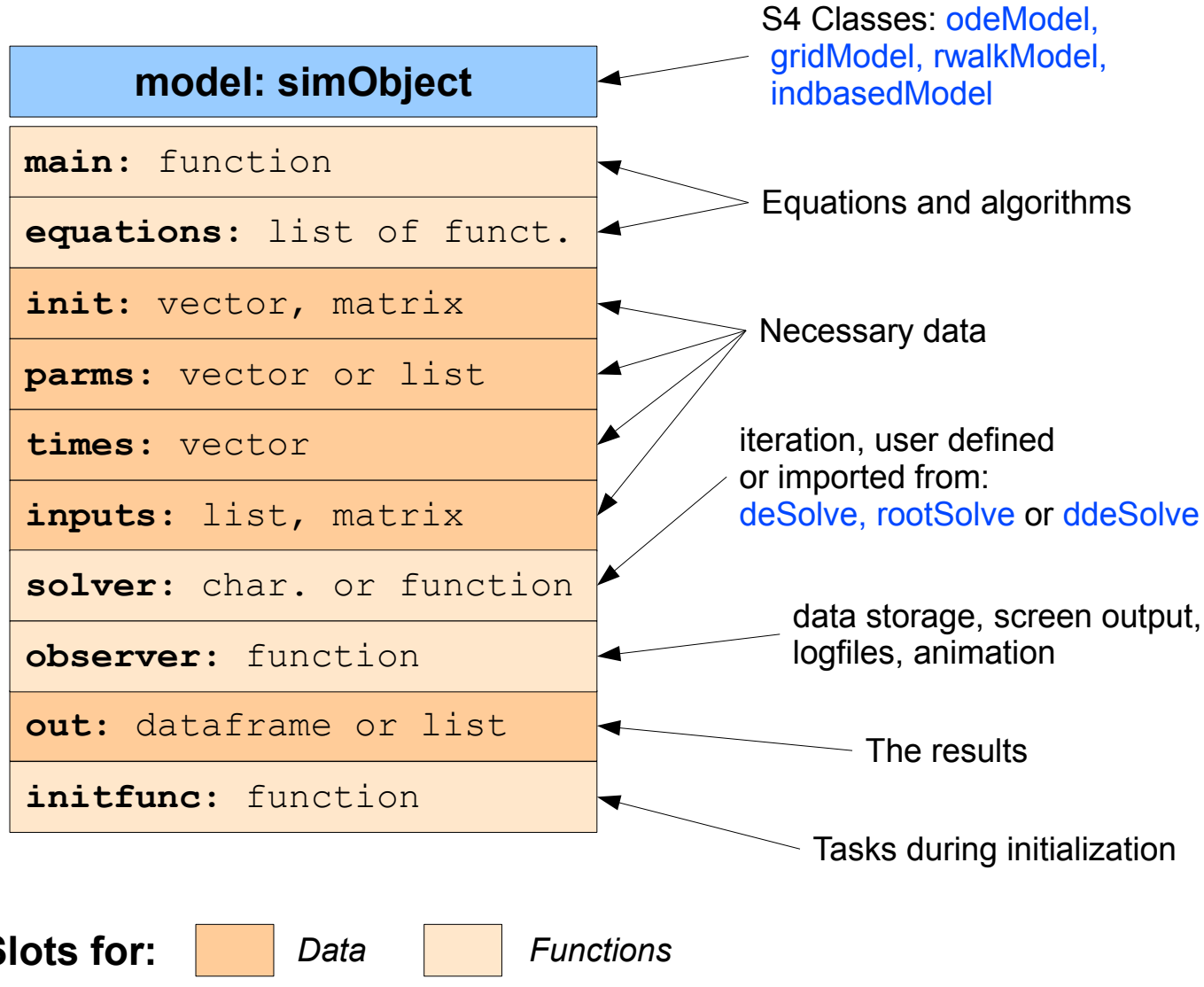
?? What do ecological / dynamic models have in common?

State Transition Diagram



Specification

A whole model in one compact object.



Example: Stochastic Cellular Automaton

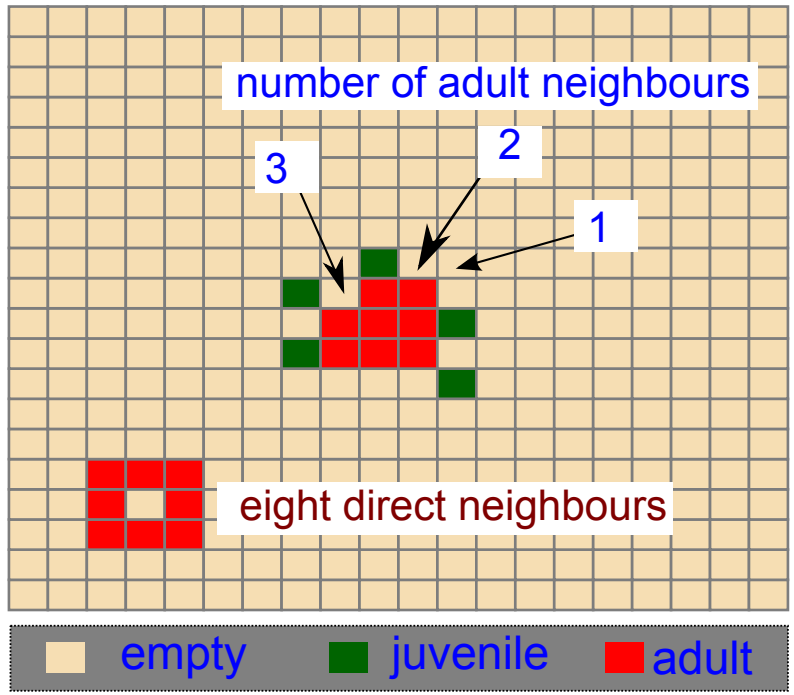
Spread of plants, animals, diseases, ...

Survival rules

- Number of direct neighbours: $n_n = n_{neighbours} \in \{0 \ldots 8\}$,
- Probability of seedling per adult neighbour: p_{seed},
- Total probability of seedlings per empty cell:

$$p_{gen} = 1 - (1 - p_{birth})^{n_n}$$

- Probability of death p_{death},
- Time step $\Delta t = 1$,
- State:
  - living cells: $Z_{i,j} = t$ (age),
  - dead cells: $Z_{i,j} = 0$.

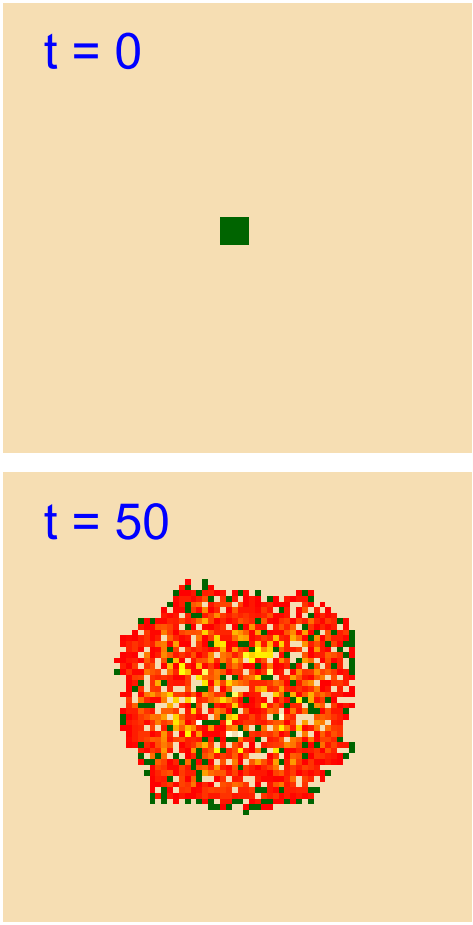


Stochastic Cellular Automaton in simecol

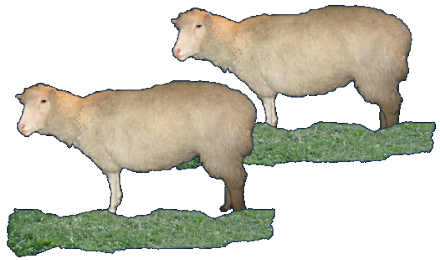
```
CA <- new('gridModel',
  main = function(time, init, parms) {
    Z <- init
    with(parms, {
      nn    <- eightneighbours(Z >= adult)   # direct neighbours
      pgen  <- 1 - (1 - pseed)^nn            # probability product
      zgen  <- ifelse(Z == 0 & runif(Z) < pgen,          1,     0)
      zsurv <- ifelse(Z >= 1 & runif(Z) < (1 - pdeath), Z + 1, 0)
      zgen + zsurv
    } )
  },
  parms = list(adult = 2, pseed = 0.2, pdeath = 0.1),
  times = c(from = 1, to = 50, by = 1),
  init = matrix(0, nrow = 80, ncol = 80),
  solver = 'iteration',
  initfunc = function(obj) {       # obj = 'object in creation'
    init(obj)[38:42, 38:42] <- 1   # ... modify it
    obj                            # return the final object.
  }
)
```

Simulate the Model

```
library('simecol')
# (1) define or load the model
# source(); data(); ...

# (2) simulate the model
# Note: pass-back modification
CA <- sim(CA)

# (3) plot the model
# ... calls a specific plot-method
plot(CA)

# (4) Extract outputs
o <- out(CA)
```



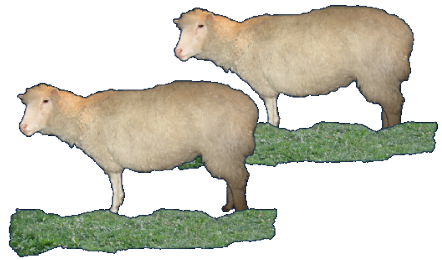
Cloning ...



Typical for Prototype-based-OOP (object-based, classless)

- Object creation: ex-nihilo or cloning and modification.
- Cloning: Creation time sharing (simple copy),
- Delegation: Run-time sharing
  (more memory efficient, but can confuse ecologists)

Cloning ...



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S4-classes not so far away from prototypes

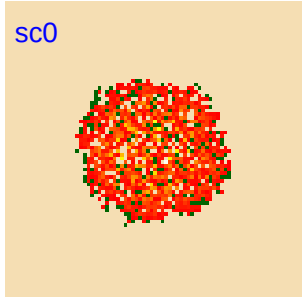
- Cloning with assignment operator

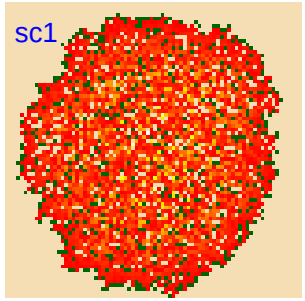
  `scenario1 <- scenario2 <- CA`

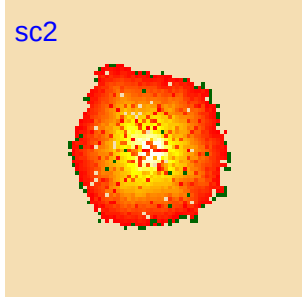
  $\Rightarrow$ Independent copies of the whole model object,
- Modify slots with replacement functions
  parms, times, initfunc, ..., equations, ...

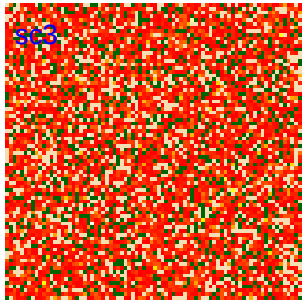
Creating Scenarios

```
# Cloning
sc0 <- sc1 <- sc2 <- sc3 <- CA

# a series of scenarios with different settings
parms(sc1)$adult <- 1          # grow-up faster
parms(sc2)$pdeath <- 0.01      # live longer

# a scenario with random initialization
initfunc(sc3) <- <- function(obj) {
  init(obj) <- matrix(round(runif(80*80)), 80, 80)
  obj
}

# (2) simulate, plot ...
plot(sim(sc0))
plot(sim(sc1))
plot(sim(sc2))
plot(sim(sc3))
```



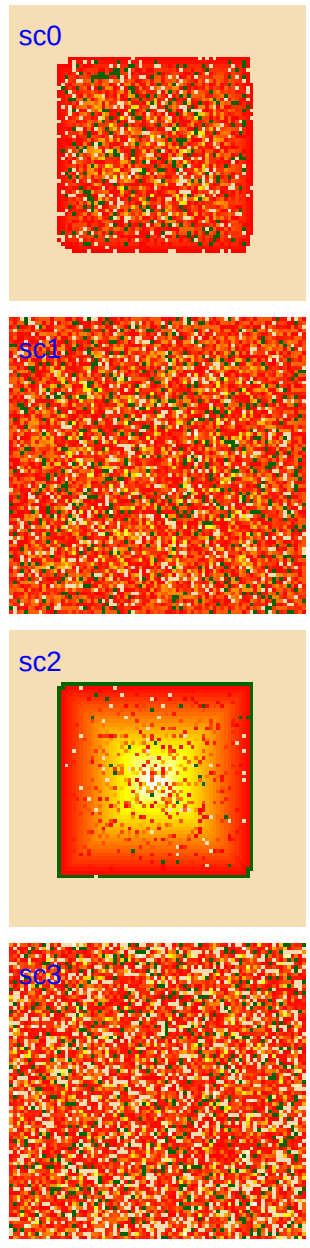






Creation-Time Sharing

```
# Cloning
sc0 <- CA                    # keep CA as backup
parms(sc0)$pseed = 1         # <-- modify sc0 globally
sc1 <- sc2 <- sc3 <- sc0

# a series of scenarios with different settings
parms(sc1)$adult <- 1
parms(sc2)$pdeath <- 0.01

# a scenario with random initialization
initfunc(sc3) <- <- function(obj) {
  init(obj) <- matrix(round(runif(80*80)), 80, 80)
  obj
}

# ... simulate, plot ...
plot(sim(sc0))
...
```



A Little Bit More Structure

The 'equations'-slot

- Modularization, functions, submodels,
- Implemented as list of functions in 'equations' (`e.g. neighb, generate, survive`)
- `main`-function should be as general as possible (call equations),

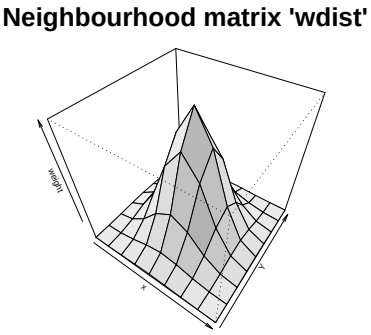
$\Rightarrow$ Possibility to derive scenarios with different functionality, e.g:

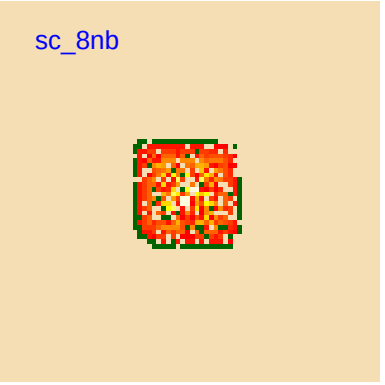
```
# 8 direct neighbours (quick and simple)
equations(sc_8nb)$neighb = function(Z, adult, ...)
  eightneighbours(Z >= adult)

# neighborhood matrix (more general)
equations(sc_wdist)$neighb <- function(Z, adult, wdist)
  neighbours(Z >= adult , wdist = wdist)
```

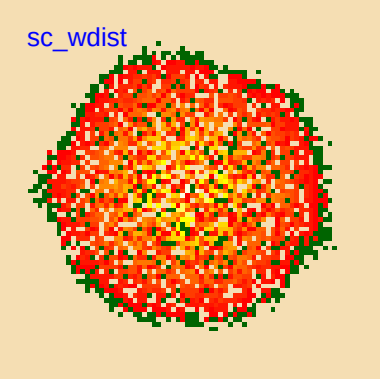
Variation of Model Structure

to compare models with different submodels

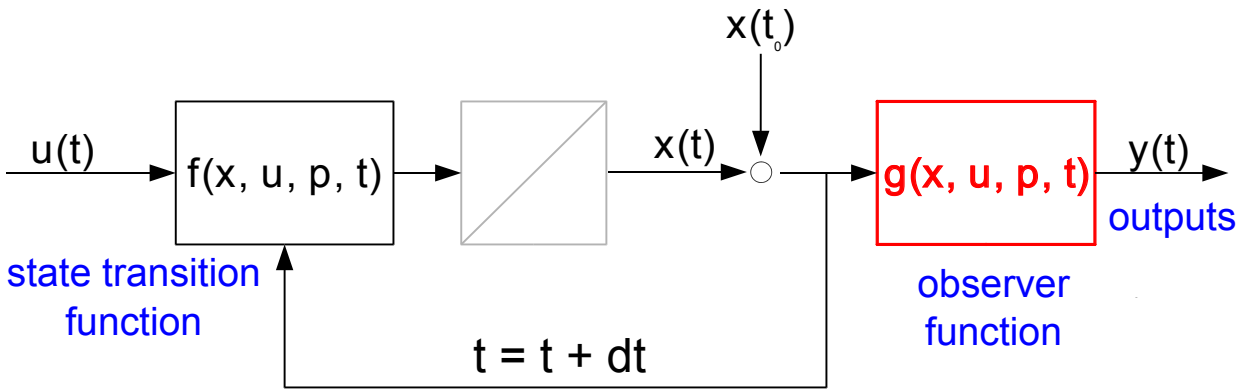
```
# A bell-shaped neighbourhood
x <- exp(-(seq(-2, 2, 0.5)^2))
parms(CA)$wdist <- outer(x, x)

# Settings for all scenarios
times(CA)['to'] <- 20
parms(CA)[c('pseed', 'pdeath')] <- c(0.9, 0.1)

# Cloning
sc_wdist <- sc_8nb <- CA

# Replace equation in scenario sc_wdist
equations(sc_wdist)$neighb <- function(Z, adult, wdist)
  neighbours(Z >= adult , wdist = wdist)

plot(sim(sc_8nb))
plot(sim(sc_wdist))
```







Observer Methods: The g in the State Transition Diagram



Purpose

- Some models produce more data than required:

⇒ Condense data, perform statistical analysis.

- Simulations can be long and "anonymous":

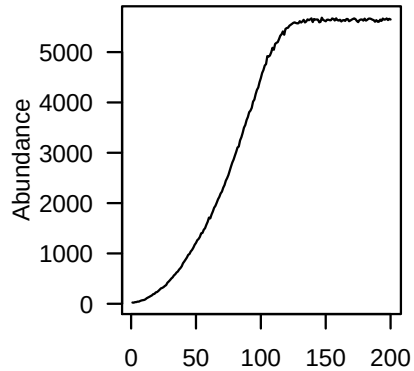
⇒ Output status info, write logfiles, show live animations.

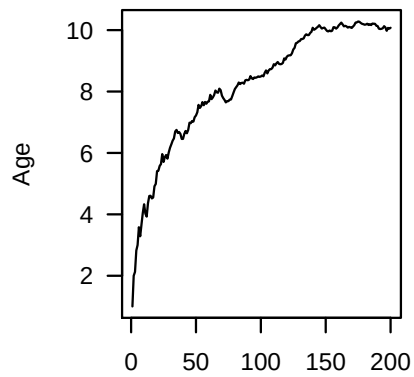
How it works

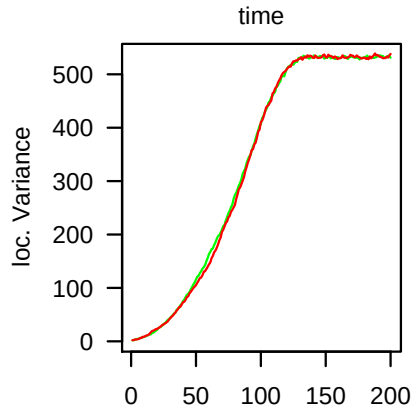
- Observer is called once in each iteration step.
- Input = state – Output = data to store in 'out'
- Alternative observers are possible for one model, e.g. minimal observer for performance or elaborated observers for demo.

Aggregating Observers

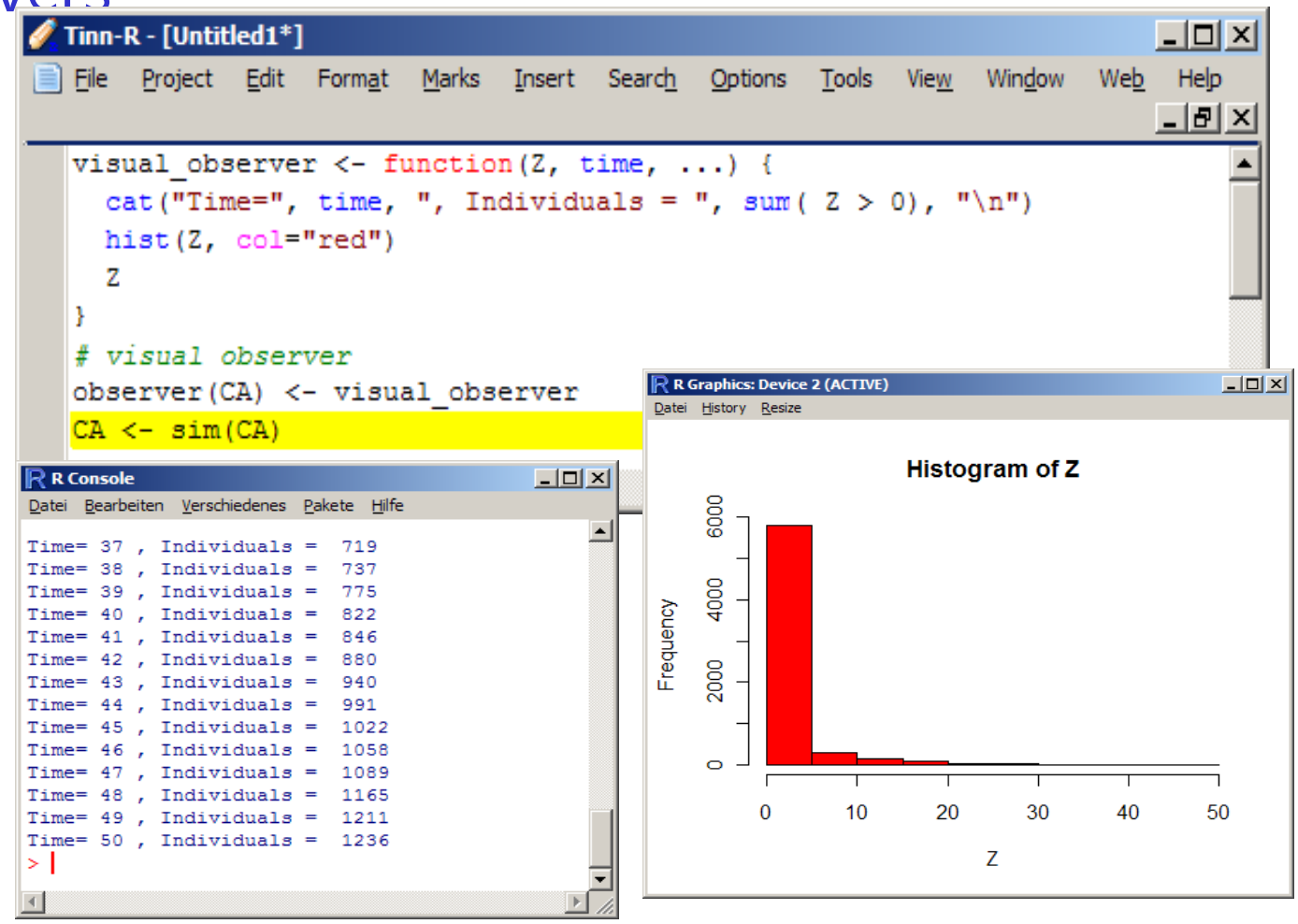
```
aggregating_observer <- function(Z, time, ...) {
  loc <- which(Z > 0, arr.ind = TRUE)
  c(abundance = sum(Z > 0), age = mean(Z[Z > 0]),
    var.x = var(loc[,1]), var.y =  var(loc[,2]))
}

# store, abundance, mean age and variances in x and y
observer(CA) <- aggregating_observer
CA <- sim(CA)
o <- out(CA)

with(o,
  plot(times, abundance)
  plot(times, age)
  plot(times, var.x, col='green')
  lines(times, var.y, col='red')
)
```







Visual Observers



- Textual output of time and abundance and
- Animated histogram of age distribution during runtime.

Outlook

Package simecol

- Suitable for playing and for serious work as well.

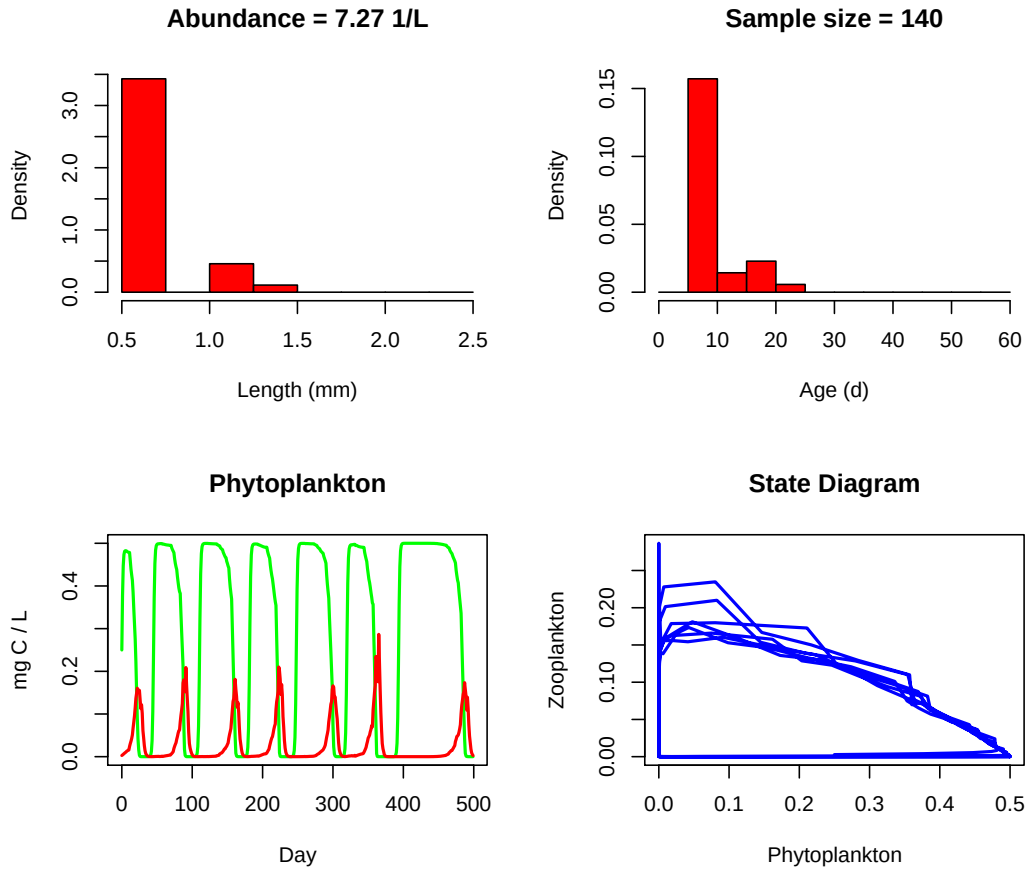
Package simecolModels[1]

- An open collection of (mostly published) models.
- Individual-based Simulation of Daphnia
  - Different versions in pure R or in R and C/C++,
  - Bioenergetic version (DEB), Cohort model (EBT),
  - Several 1000 individuals possible.
- Models for Marine Systems (among them 2D)
  - Use new differential equation solvers (package deSolve)
  - Thanks to Karline Soetaert[2], NIOO, NL
- . . . and more.

[1] www.simecol.de, development on R-Forge

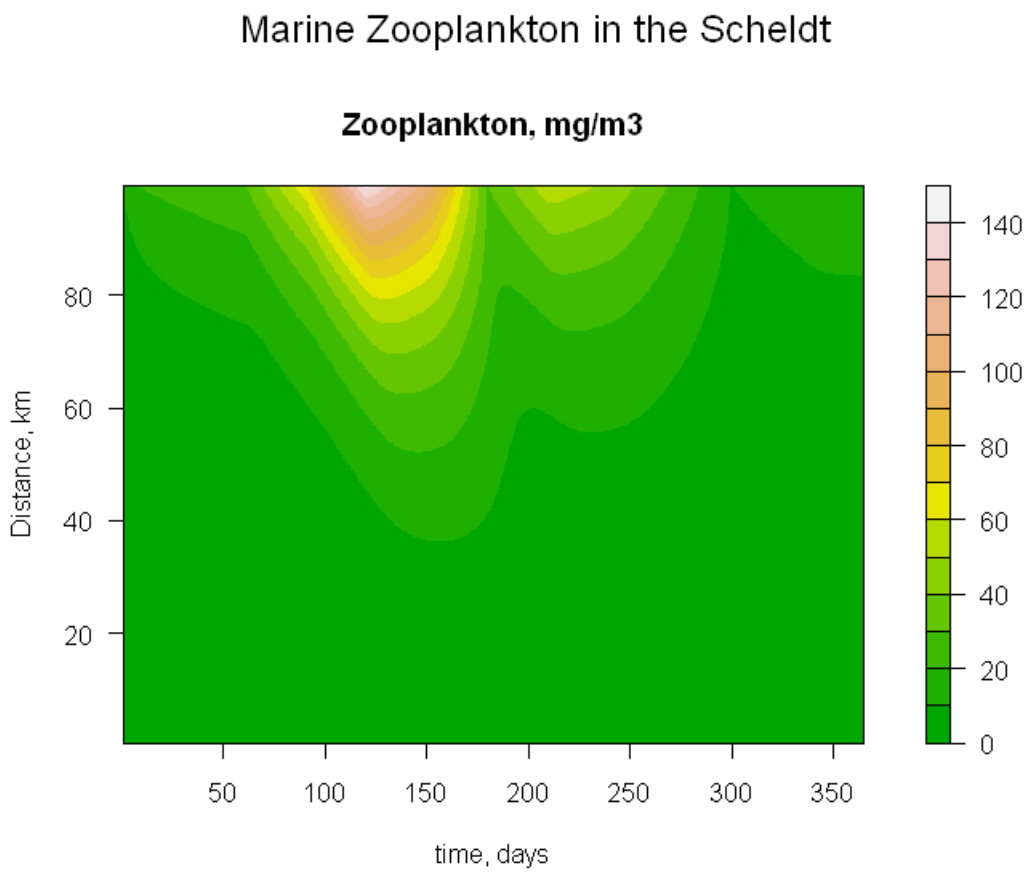
[2] Note her upcoming book about practical ecological modelling in R.

One of Our Daphnia models



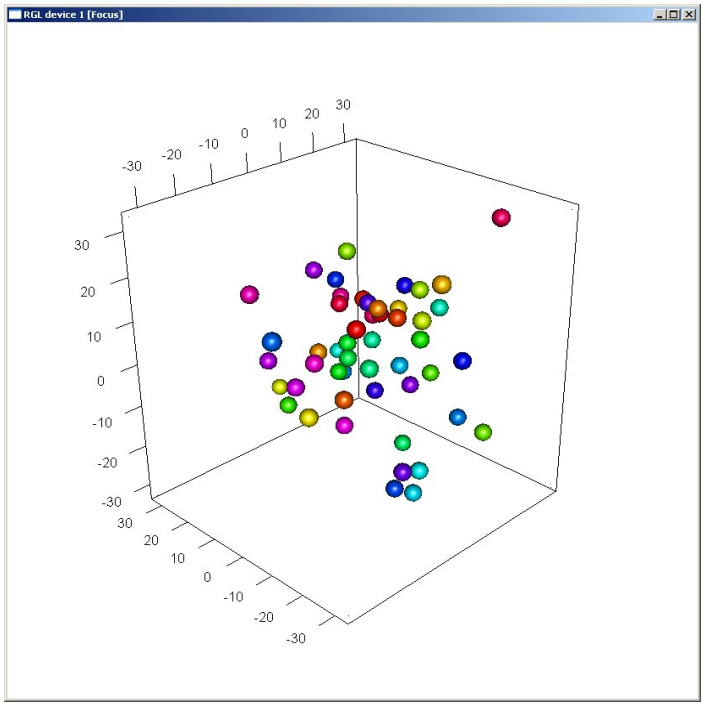
- Individual-based in R, bioenergetic core model in C/C++
- Live animation

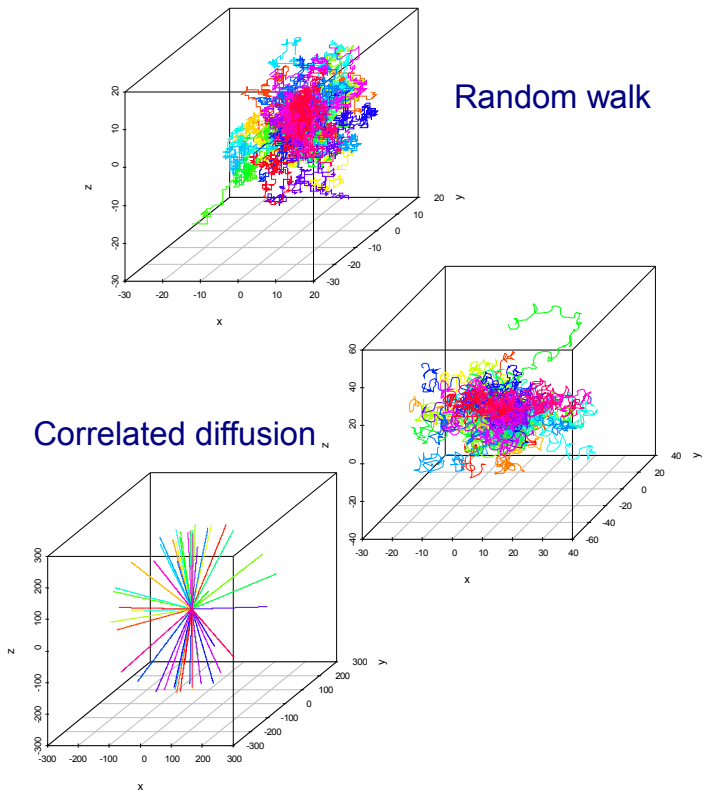
A Horizontal 2D Zooplankton Model



- Partial differential equation (PDE) model,
- Available in simecolModels,
- Soetaert and Herman, 1994. Marine Ecology Progress Series 105: 19-29.

Random Walk Model in 3D





Live animation with RGL

- implemented as observer method

```
library(simecol); demo(rwalk3d)
```

- A live demo is possible – if you like ...

Conclusions: Why using simecol?

Pre-defined structure:

- Compact, standardized representation of models,
- Improved readability (your code and that of your students).

Scenario control made easy:

- Formalized Cloning instead of cumbersome copy & paste,
- Standard methods for changing data and formula,
- No interference between different instances of one model.

Reproducible Science:

- Model input and outcome together in one object,
- Objects can be stored in binary or human readable form.

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Reproducible Science:

- Model input and outcome together in one object,
- Objects can be stored in binary or human readable form.

$\Rightarrow$ simecol-Models: a nice gift for your friends.

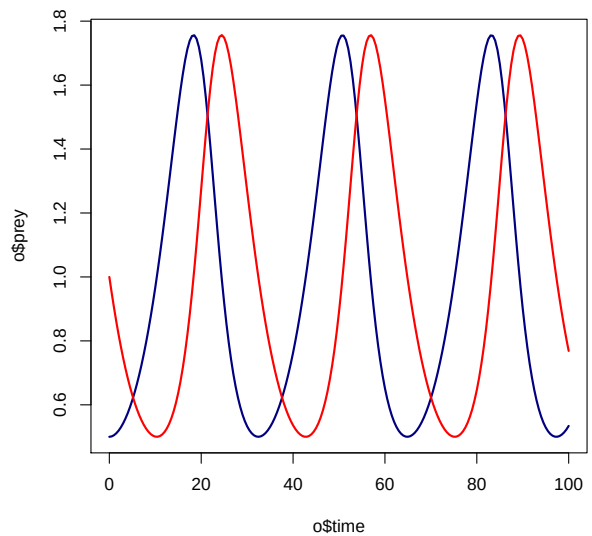
Appendix

One simple example

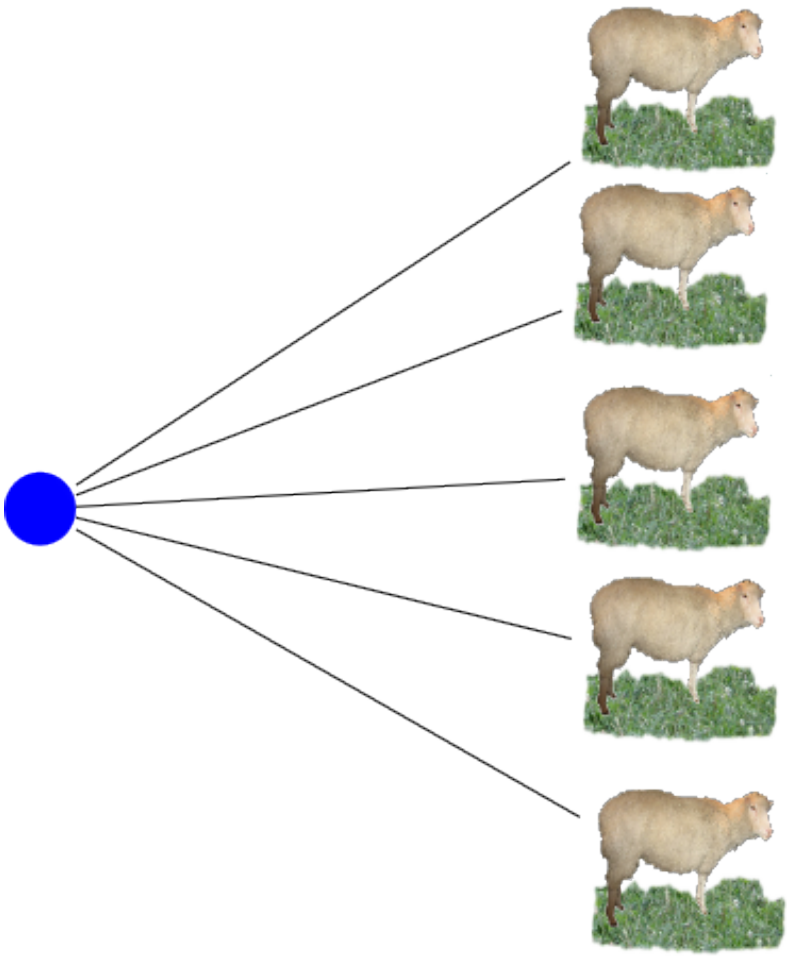
Lotka-Volterra-Model

```
lv <- new('odeModel',
  main = function (time, init, parms) {
    x <- init
    with(as.list(parms), {
      dx1 <-   b * x[1] - e * x[1] * x[2]
      dx2 <- - d * x[2] + e * x[1] * x[2]
      list(c(dx1, dx2))
    })
  },
  ##          birth encounter death
  parms  = c(b=0.2, e=0.2, d=0.2),
  times  = seq(0, 100, 1),
  init   = c(prey=0.5, predator=1)
)

plot(sim(lv))
```

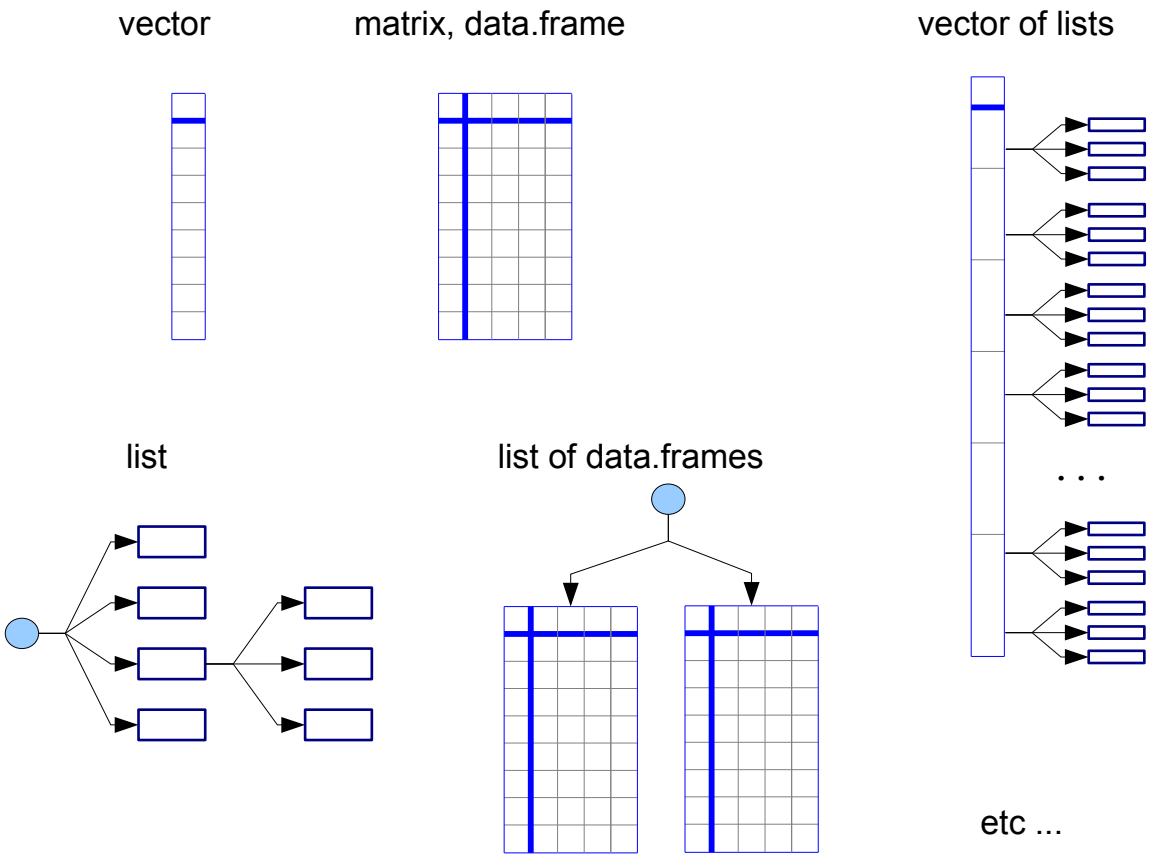


Agent based models (ABMs) with R?



Data structures in R

Object oriented, high-level, performance-optimzed



- "Large Blocks" $\Rightarrow$ good Performance.
- Time critical code $\longrightarrow$ C/C++, Fortran or JAVA.

Contact Information

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http://www.simecol.de

Clone sheep picture:
http://commons.wikimedia.org/wiki/Image:Dollyscotland_(crop).jpg

The examples were created with R 2.7.1, simecol 0.6 and simecolModels 0.2-3. Full source code of the examples is part of these packages.

To cite package 'simecol' in publications, please use:

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