Differential Equations in R

Tutorial useR conference 2011

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Outline

- How to specify a model
- An overview of solver functions
- Plotting, scenario comparison,
- Fitting models to data,

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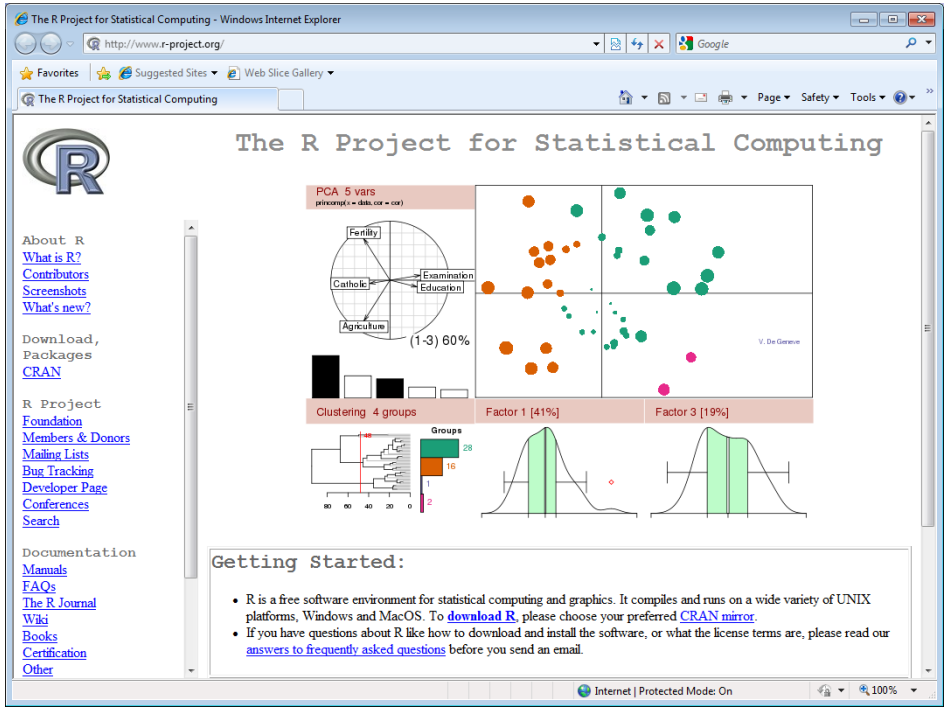
- How to specify a model
- An overview of solver functions
- Plotting, scenario comparison,
- Fitting models to data,

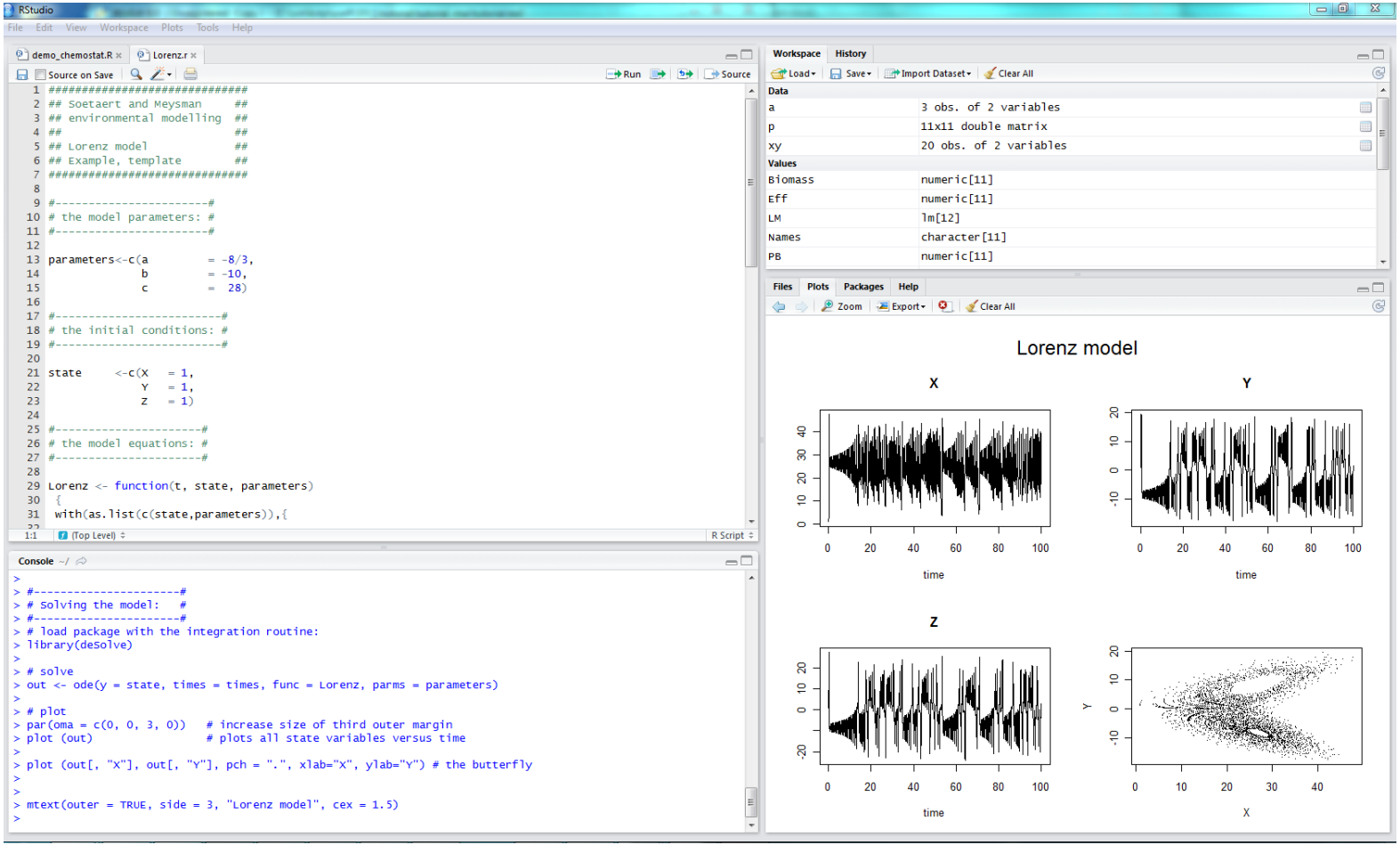
- Forcing functions and events
- Partial differential equations with ReacTran
- Speeding up

Download R from the CRAN website: http://cran.r-project.org/

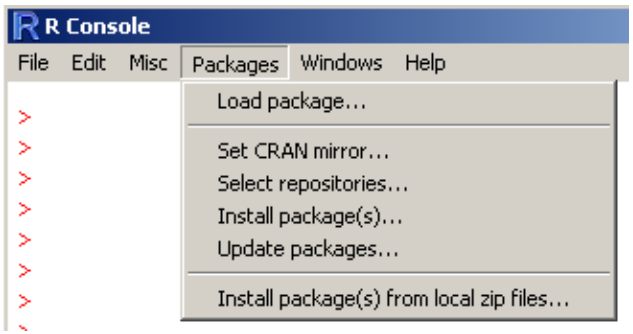


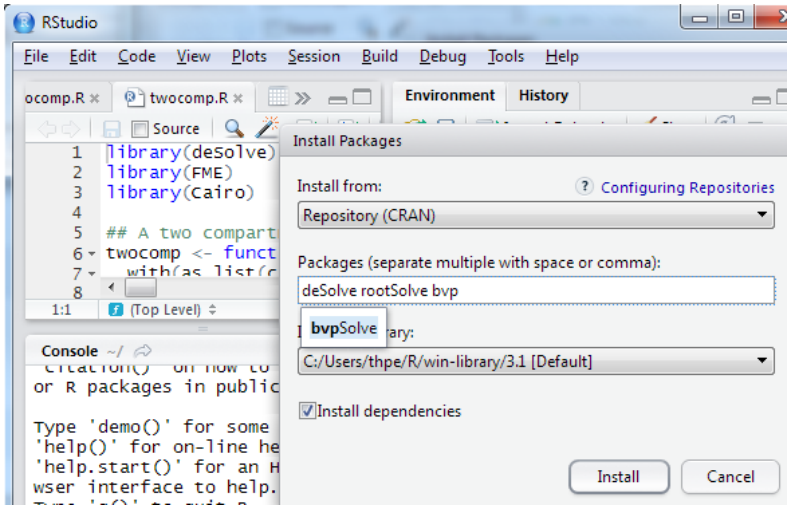
Install a suitable editor

. . . e.g. RStudio



Packages can be installed from within R or Rstudio:





. . . or via the command line

```
install.packages("deSolve", dependencies = TRUE)
```

Several packages deal with differential equations

- deSolve: main integration package
- rootSolve: steady-state solver
- bvpSolve: boundary value problem solvers
- deTestSet: ODE and DAE test set + additional solvers
- ReacTran: partial differential equations
- simecol: interactive environment for implementing models

All packages have at least one author in common → consistent interface.

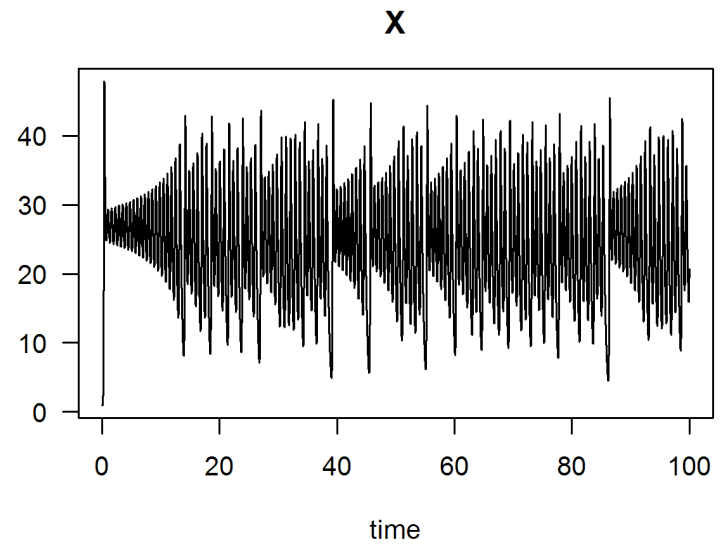
More, see CRAN Task View: Differential Equations

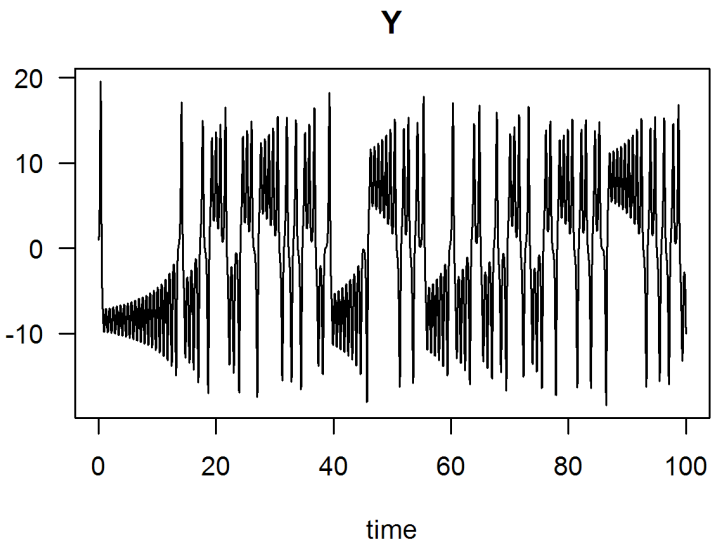
Getting help

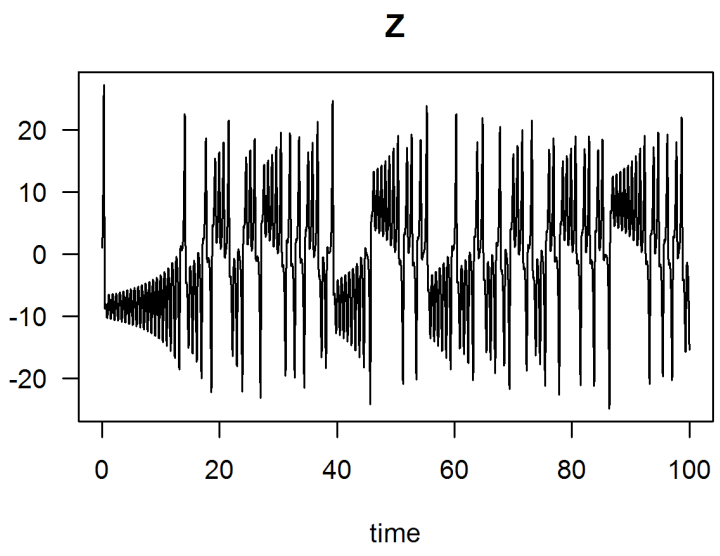
```
> library(deSolve)
> ?deSolve
```

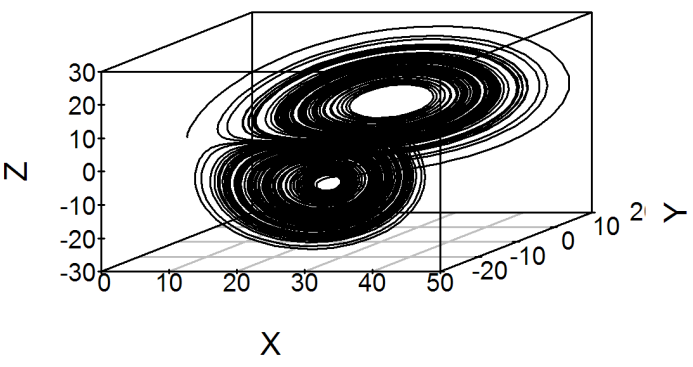
- opens the main help page containing
  - a short explanation
  - a link to the main manual (vignette)
    "Solving Initial Value Differential Equations in R"
  - links to additional manuals, papers and online resources
  - references
  - a first example
- all our packages have such a ?<packagename> help file.

```
> library(deSolve)
> example(deSolve)
```









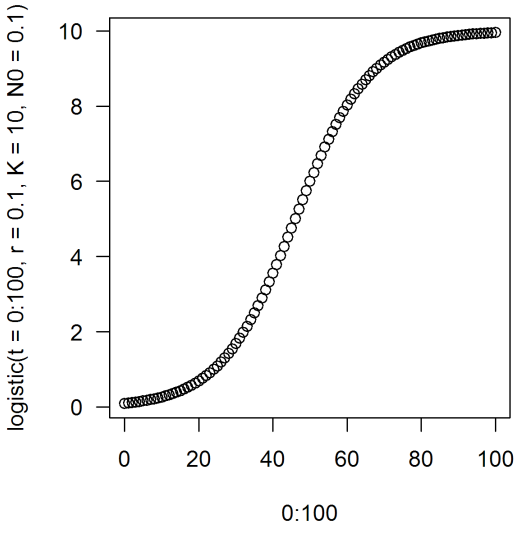
Let's begin ...

Model specification

Logistic growth

Differential equation

$$\frac{dN}{dt} = r \cdot N \cdot \left(1 - \frac{N}{K}\right)$$



Analytical solution

$$N_t = \frac{K N_0 e^{rt}}{K + N_0 \left(e^{rt} - 1\right)}$$

R implementation

```
> logistic <- function(t, r, K, N0) {
+   K * N0 * exp(r * t) / (K + N0 * (exp(r * t) - 1))
+ }
> plot(0:100, logistic(t = 0:100, r = 0.1, K = 10, N0 = 0.1))
```

Numerical simulation in R

Why numerical solutions?

- Not all systems have an analytical solution,
- Numerical solutions allow discrete forcings, events, ...

Why R?

- If standard tool for statistics, why Prog$$$ for dynamic simulations?
- The community and the packages $\rightarrow$ useR!2014

Numerical solution of the logistic equation

http://desolve.r-forge.r-project.org

```
library(deSolve)
model <- function (time, y, parms) {
  with(as.list(c(y, parms)), {
    dN <-   r * N * (1 - N / K)
    list(dN)
  })
}

y      <- c(N = 0.1)
parms  <- c(r = 0.1, K = 10)
times  <- seq(0, 100, 1)

out <- ode(y, times, model, parms)

plot(out)
```

Differential equation
„similar to formula on paper"

Numerical methods provided by the deSolve package

Inspecting output

- Print to screen

```
> head(out, n = 4)
```

```
     time         N
[1,]    0 0.1000000
[2,]    1 0.1104022
[3,]    2 0.1218708
[4,]    3 0.1345160
```

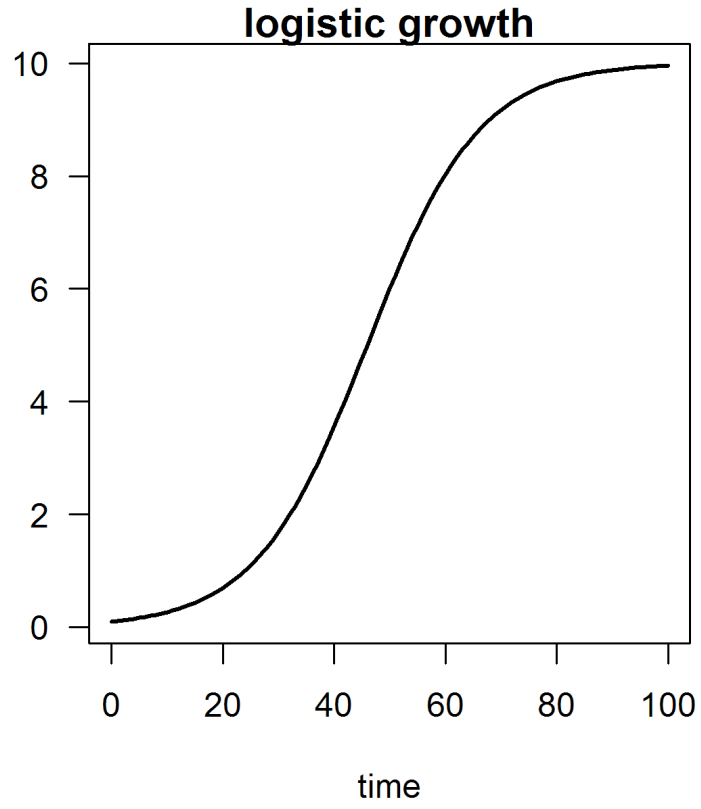
- Summary

```
> summary(out)
```

```
                      N
Min.          0.100000
1st Qu.       1.096000
Median        5.999000
Mean          5.396000
3rd Qu.       9.481000
Max.          9.955000
N           101.000000
sd            3.902511
```

- Plotting

```
> plot(out, main = "logistic growth", lwd = 2)
```



> diagnostics(out)

```
-------------------
lsoda return code
-------------------

  return code (idid) =  2
  Integration was successful.

-------------------
INTEGER values
-------------------

  1 The return code : 2
  2 The number of steps taken for the problem so far: 105
  3 The number of function evaluations for the problem so far: 211
  5 The method order last used (successfully): 5
  6 The order of the method to be attempted on the next step: 5
  7 If return flag =-4,-5: the largest component in error vector 0
  8 The length of the real work array actually required: 36
  9 The length of the integer work array actually required: 21
 14 The number of Jacobian evaluations and LU decompositions so far: 0
 15 The method indicator for the last succesful step,
           1=adams (nonstiff), 2= bdf (stiff): 1
 16 The current method indicator to be attempted on the next step,
           1=adams (nonstiff), 2= bdf (stiff): 1

-------------------
RSTATE values
```

Coupled ODEs: the rigidODE problem

Problem

- Euler equations of a rigid body without external forces.
- Three dependent variables (y_1, y_2, y_3), the coordinates of the rotation vector,
- I_1, I_2, I_3 are the principal moments of inertia.

[3] E. Hairer, S. P. Norsett, and G Wanner. Solving Ordinary Differential Equations I: Nonstiff Problems. Second Revised Edition. Springer-Verlag, Heidelberg, 2009

Coupled ODEs: the rigidODE equations

Differential equation

$$\begin{aligned} y_1' &= (I_2 - I_3)/I_1 \cdot y_2 y_3 \\ y_2' &= (I_3 - I_1)/I_2 \cdot y_1 y_3 \\ y_3' &= (I_1 - I_2)/I_3 \cdot y_1 y_2 \end{aligned}$$

Parameters

$$I_1 = 0.5, I_2 = 2, I_3 = 3$$

Initial conditions

$$y_1(0) = 1, y_2(0) = 0, y_3(0) = 0.9$$

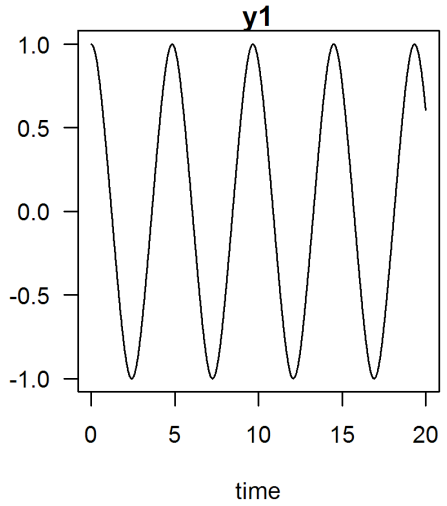
Coupled ODEs: the rigidODE problem

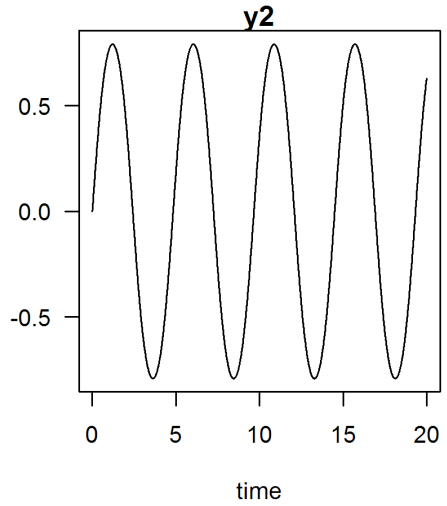
R implementation

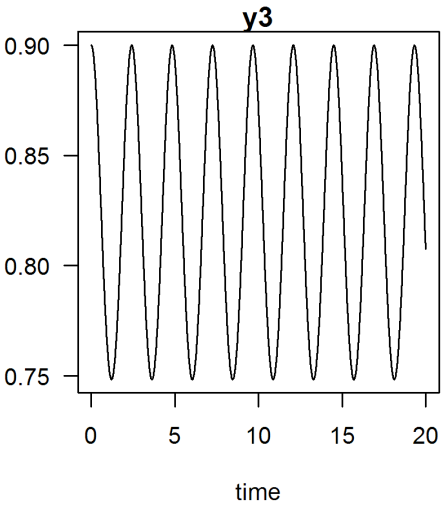
```
> library(deSolve)
> rigidode <- function(t, y, parms) {
+   dy1 <- -2   * y[2] * y[3]
+   dy2 <- 1.25 * y[1] * y[3]
+   dy3 <- -0.5 * y[1] * y[2]
+   list(c(dy1, dy2, dy3))
+ }
> yini  <- c(y1 = 1, y2 = 0, y3 = 0.9)
> times <- seq(from = 0, to = 20, by = 0.01)
> out   <- ode (times = times, y = yini, func = rigidode, parms = NULL)

> head (out, n = 3)

     time        y1         y2        y3
[1,] 0.00 1.0000000 0.00000000 0.9000000
[2,] 0.01 0.9998988 0.01124925 0.8999719
[3,] 0.02 0.9995951 0.02249553 0.8998875
```

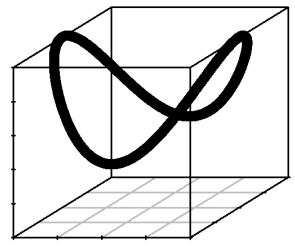
Coupled ODEs: plotting the rigidODE problem

```
> plot(out)
> library(scatterplot3d)
> par(mar = c(0, 0, 0, 0))
> scatterplot3d(out[,-1])
```









Exercise

The Rössler equations

$$\begin{aligned} y_1' &= -y_2 - y_3 \\ y_2' &= y_1 + a \cdot y_2 \\ y_3' &= b + y_3 \cdot (y_1 - c) \end{aligned}$$

Initial Conditions

$$y_1 = 1, y_2 = 1, y_3 = 1$$

Parameters

$$a = 0.2, b = 0.2, c = 5$$

Tasks

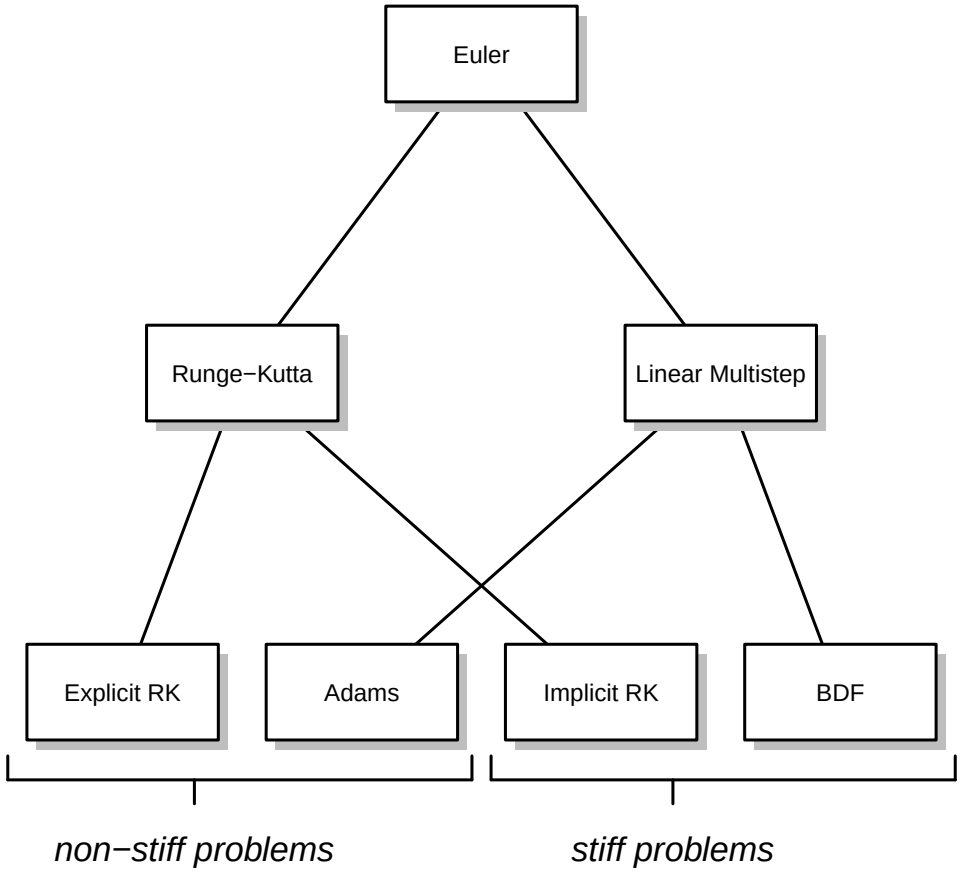
- Solve the ODEs on the interval $[0, 100]$
- Produce a 3-D phase-plane plot
- Use file `examples/rigidODE.R.txt` as a template

[13] O.E. Rössler. An equation for continous chaos. Physics Letters A, 57 (5):397-398, 1976.

Solvers ...

Solver overview, stiffness, accuracy

Integration methods: package deSolve [22]



Solver overview: package deSolve

Solver	Notes	stiff	y'=f(t,y)	My'=f(t,y)	F(y',t,y)=0	Roots	Events	Lags (DDE)	Nesting
lsoda/lsodar	automatic method selection	auto	x			x	x	x	
lsode	bdf, adams, …	user defined	x			x	x	x	
lsodes	sparse Jacobian	yes	x			x	x	x	
vode	bdf, adams, …	user defined	x				x	x	
zvode	complex numbers	user defined	x				x	x	
daspk	DAE solver	yes	x	x	x		x	x	
radau	DAE; implicit RK	yes	x	x		x	x	x	
rk, rk4, euler	euler, ode23, ode45, … rkMethod	no	x				x		x
iteration	returns state at t+dt	no	x				x		x

- ode, ode.band, ode.1D, ode.2D, ode.3D: top level functions (wrappers)
- red: functionality added by us

adapte

Options of solver functions

Top level function

```
> ode(y, times, func, parms,
+   method = c("lsoda", "lsode", "lsodes", "lsodar", "vode", "daspk",
+              "euler", "rk4", "ode23", "ode45", "radau",
+              "bdf", "bdf_d", "adams", "impAdams", "impAdams_d",
+              "iteration"), ...)
```

Workhorse function: the individual solver

```
> lsoda(y, times, func, parms, rtol = 1e-6, atol = 1e-6,
+   jacfunc = NULL, jactype = "fullint", rootfunc = NULL,
+   verbose = FALSE, nroot = 0, tcrit = NULL,
+   hmin = 0, hmax = NULL, hini = 0, ynames = TRUE,
+   maxordn = 12, maxords = 5, bandup = NULL, banddown = NULL,
+   maxsteps = 5000, dllname = NULL, initfunc = dllname,
+   initpar = parms, rpar = NULL, ipar = NULL, nout = 0,
+   outnames = NULL, forcings = NULL, initforc = NULL,
+   fcontrol = NULL, events = NULL, lags = NULL,...)
```

Arghhh, which solver and which options???

Problem type?

- ODE: use `ode`,
- DDE: use `dede`,
- DAE: `daspk` or `radau`,
- PDE: `ode.1D, ode.2D, ode.3D`,

...others for specific purposes, e.g. root finding, difference equations (`euler, iteration`) or just to have a comprehensive solver suite (`rk4, ode45`).

Stiffness

- default solver `lsoda` selects method automatically,
- `adams` or `bdf` may speed up a little bit if degree of stiffness is known,
- `vode` or `radau` may help in difficult situations.

Solvers for stiff systems

Stiffness

- Difficult to give a precise definition.

≈ system where some components change more rapidly than others.

Sometimes difficult to solve:

- solution can be numerically unstable,
- may require very small time steps (slow!),
- deSolve contains solvers that are suitable for stiff systems,

But: "stiff solvers" slightly less efficient for "well behaving" systems.

- **Good news**: `lsoda` selects automatically between stiff solver (bdf) and nonstiff method (adams).

Van der Pol equation

Oscillating behavior of electrical circuits containing tubes [24].

2^{nd} order ODE

$$y'' - \mu(1 - y^2)y' + y = 0$$

. . . must be transformed into two 1^{st} order equations

$$y_1' = y_2$$
$$y_2' = \mu \cdot (1 - {y_1}^2) \cdot y_2 - y_1$$

- Initial values for state variables at $t = 0$: $y_{1_{(t=0)}} = 2, y_{2_{(t=0)}} = 0$
- One parameter: μ = large $\rightarrow$ stiff system; μ = small $\rightarrow$ non-stiff.

Model implementation

```
> library(deSolve)
> vdpol <- function (t, y, mu) {
+   list(c(
+           y[2],
+           mu * (1 - y[1]^2) * y[2] - y[1]
+   ))
+ }

> yini <- c(y1 = 2, y2 = 0)

> stiff <- ode(y = yini, func = vdpol, times = 0:3000, parms = 1000)
> nonstiff <- ode(y = yini, func = vdpol, times = seq(0, 30, 0.01), parms = 1)

> head(stiff, n = 5)

     time       y1            y2
[1,]    0 2.000000  0.0000000000
[2,]    1 1.999333 -0.0006670373
[3,]    2 1.998666 -0.0006674088
[4,]    3 1.997998 -0.0006677807
[5,]    4 1.997330 -0.0006681535
```

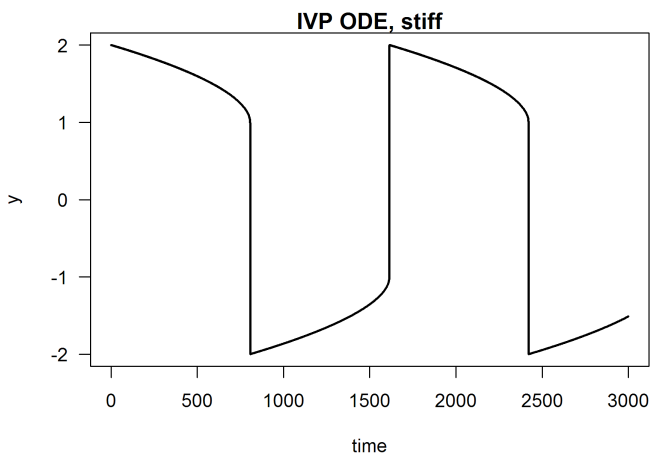
Interactive exercise

- The following link opens in a web browser. It requires a recent version of Firefox or Chrome, ideally in full-screen mode. Use Cursor keys for slide transition:
- **Left cursor** guides you through the full presentation.
- **Mouse** and **mouse wheel** for full-screen panning and zoom.
- **Pos1** brings you back to the first slide.
  - `examples/vanderpol/vanderpol.svg`
- The following opens the code as text file for life demonstrations in R
  - `examples/vanderpol/vanderpol.R.txt`

Plotting

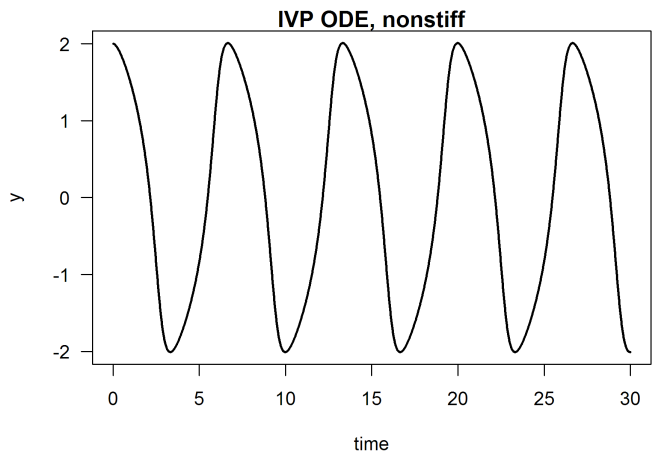
Stiff solution

```
> plot(stiff, type = "l", which = "y1",
+      lwd = 2, ylab = "y",
+      main = "IVP ODE, stiff")
```



Nonstiff solution

```
> plot(nonstiff, type = "l", which = "y1",
+      lwd = 2, ylab = "y",
+      main = "IVP ODE, nonstiff")
```



Default solver, `lsoda`:

```
> system.time(
+   stiff <- ode(yini, 0:3000, vdpol, parms = 1000)
+ )

   user  system elapsed
   0.11    0.00    0.11

> system.time(
+   nonstiff <- ode(yini, seq(0, 30, by = 0.01), vdpol, parms = 1)
+ )

   user  system elapsed
   0.09    0.00    0.09
```

Implicit solver, `bdf`:

```
> system.time(
+   stiff <- ode(yini, 0:3000, vdpol, parms = 1000,  method = "bdf")
+ )

   user  system elapsed
   0.09    0.00    0.09

> system.time(
+   nonstiff <- ode(yini, seq(0, 30, by = 0.01), vdpol, parms = 1, method = "bdf")
+ )

   user  system elapsed
   0.04    0.00    0.05
```

$\Rightarrow$ Now use other solvers, e.g. `adams`, `ode45`, `radau`.

Results

Timing results; your computer may be faster:

solver	non-stiff	stiff
ode23	0.37	271.19
lsoda	0.26	0.23
adams	0.13	616.13
bdf	0.15	0.22
radau	0.53	0.72

Comparison of solvers for a stiff and a non-stiff parametrisation of the van der Pol equation (time in seconds, mean values of ten simulations on my old AMD X2 3000 CPU).

Accuracy and stability

- Options `atol` and `rtol` specify accuracy,
- Stability can be influenced by specifying `hmax` and `maxsteps`.

Accuracy and stability - ctd

atol (default 10^{-6}) defines absolute threshold,

- select appropriate value, depending of the size of your state variables,
- may be between $\approx 10^{-300}$ (or even zero) and $\approx 10^{300}$.

rtol (default 10^{-6}) defines relative threshold,

- It makes no sense to specify values $< 10^{-15}$ because of the limited numerical resolution of double precision arithmetics ($\approx$ 16 digits).

hmax is automatically set to the largest difference in times, to avoid that the simulation possibly ignores short-term events. Sometimes, it may be set to a smaller value to improve robustness of a simulation.

hmin should normally not be changed.

Example: Setting rtol and atol: `examples/PCmod_atol_0.R.txt`

Plotting, scenario comparison, observations

Plotting and printing

Methods for plotting and extracting data in deSolve

- `subset` extracts specific variables that meet certain constraints.
- `plot`, `hist` create one plot per variable, in a number of panels
- `image` for plotting 1-D, 2-D models
- `plot.1D` and `matplot.1D` for plotting 1-D outputs

- `?plot.deSolve` opens the main help file

rootSolve has similar functions

- `subset` extracts specific variables that meet certain constraints.
- `plot` for 1-D model outputs, `image` for plotting 2-D, 3-D model outputs

- `?plot.steady1D` opens the main help file

The Lorenz equations

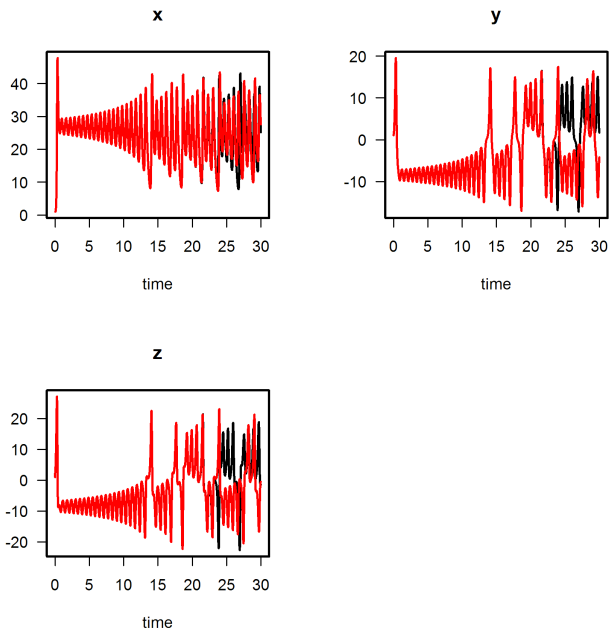
- chaotic dynamic system of ordinary differential equations
- three variables, X, Y and Z represent idealized behavior of the earth's atmosphere.

```
> chaos <- function(t, state, parameters) {
+   with(as.list(c(state)), {
+     dx     <- -8/3 * x + y * z
+     dy     <- -10 * (y - z)
+     dz     <- -x * y + 28 * y - z
+     list(c(dx, dy, dz))
+   })
+ }
> yini  <- c(x = 1, y = 1, z = 1)
> yini2 <- yini + c(1e-6, 0, 0)
> times <- seq(0, 30, 0.01)
> out  <- ode(y = yini, times = times, func = chaos, parms = 0)
> out2 <- ode(y = yini2, times = times, func = chaos, parms = 0)
```

Plotting multiple scenarios

- The default for plotting one or more objects is a line plot
- We can plot as many objects of class `deSolve` as we want
- By default different outputs get different colors and line types

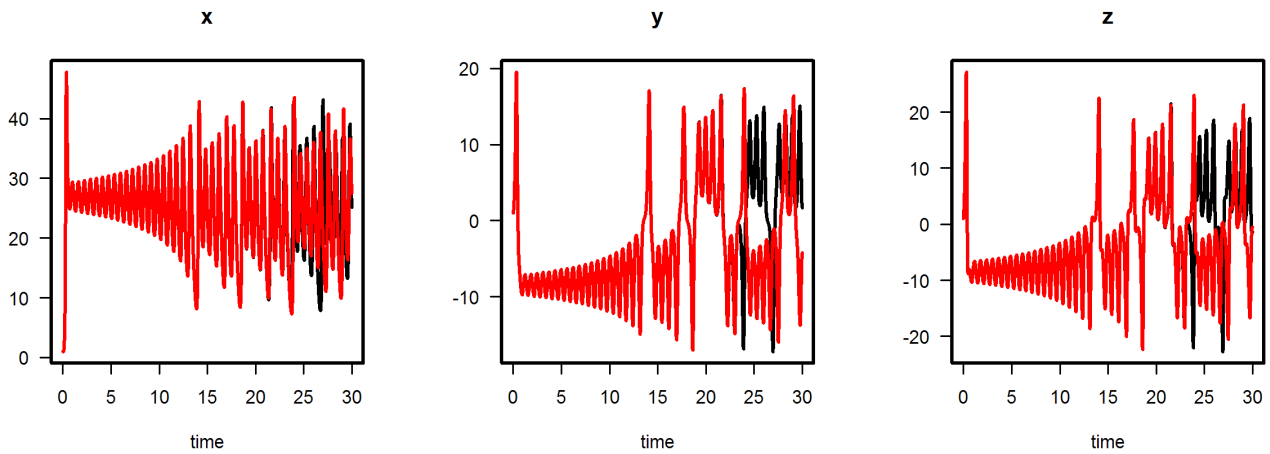
```
> plot(out, out2, lwd = 2, lty = 1)
```



Changing the panel arrangement

- Default: Automatic number of panels per page up to 3 x 3
- Use `mfrow()` or `mfcol()` to overrule

```
> plot(out, out2, lwd = 2, lty = 1, mfrow = c(1, 3))
```

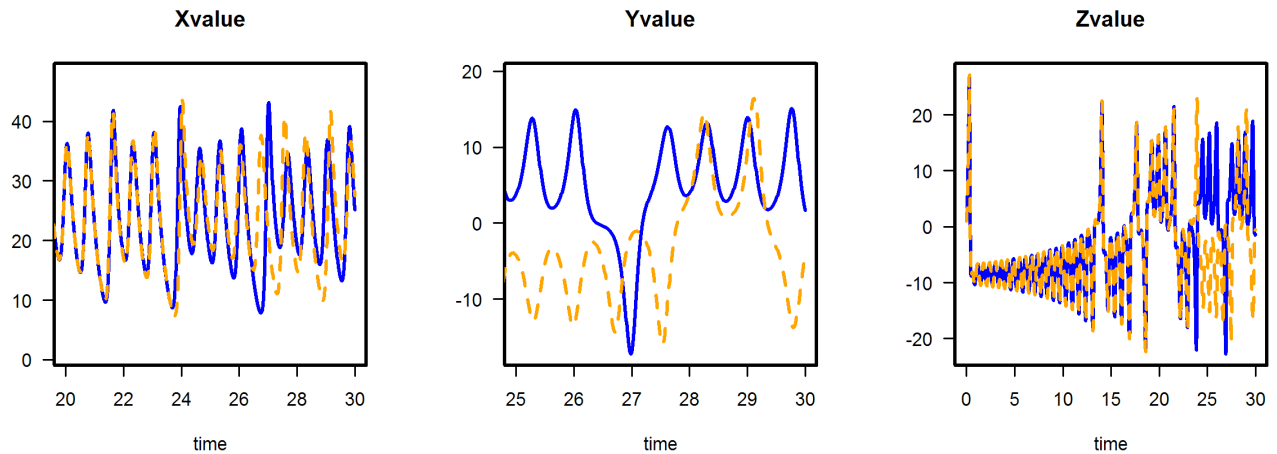


- Important: upon returning the default `mfrow` is NOT restored.

Plotting style

- We can change the style of the *dataseries* (`col`, `lty`, ...)
  - will be effective for all figures
- We can change individual *figure* settings (`title`, labels, ...)
  - vector input can be specified by a list; `NULL` will select the default

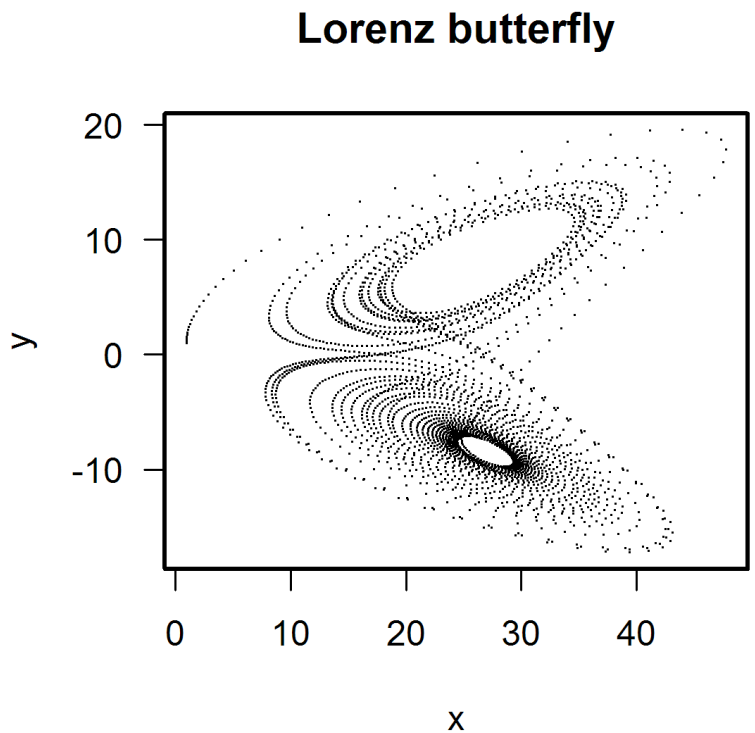
```
> plot(out, out2, col = c("blue", "orange"),
+      main = c("Xvalue", "Yvalue", "Zvalue"),
+      xlim = list(c(20, 30), c(25, 30), NULL), mfrow = c(1, 3))
```



R's default plot ...

is used if we extract single colums from the deSolve object

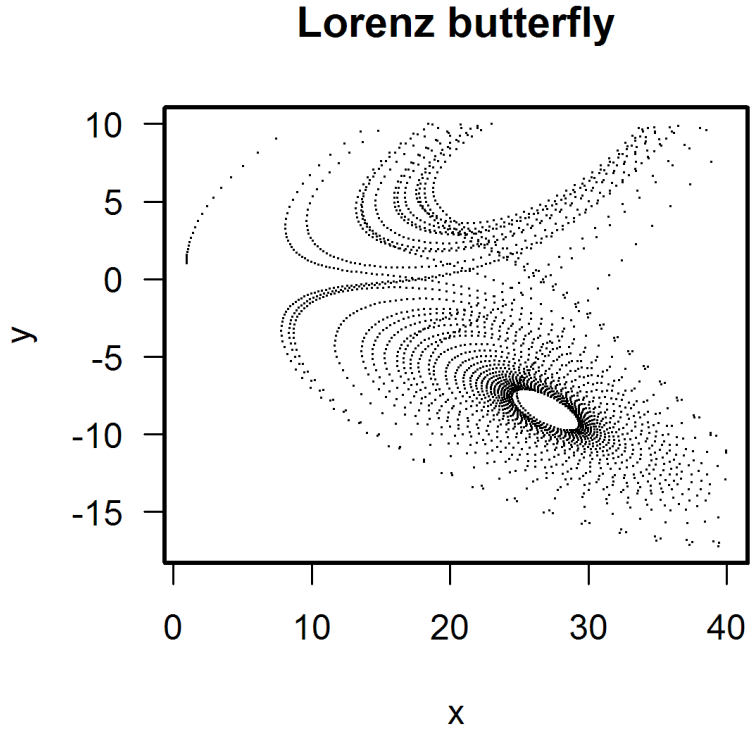
```
> plot(out[,"x"], out[,"y"], pch = ".", main = "Lorenz butterfly",
+      xlab = "x", ylab = "y")
```



Use deSolve's subset . . .

. . . to select values that meet certain conditions

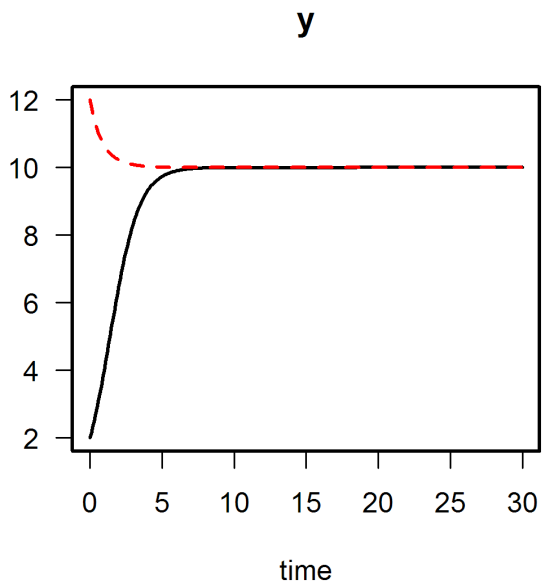
```
> XY <- subset(out, select = c("x", "y"), subset = y < 10 & x < 40)
> plot(XY, main = "Lorenz butterfly", xlab = "x", ylab = "y", pch = "."
```



Plotting multiple scenarios . . .

. . . is simple if number of outputs is known

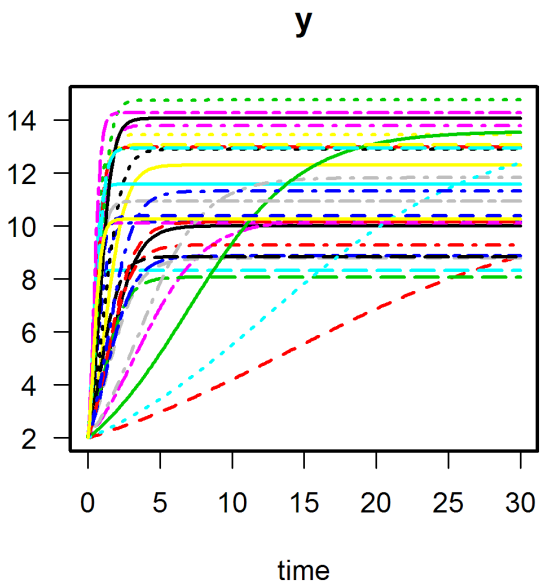
```
> derivs <- function(t, y, parms)
+    with (as.list(parms), list(r * y * (1 - y/K)))
> times <- seq(from = 0, to = 30, by = 0.1)
> out   <- ode(y = c(y =  2), times, derivs, parms = c(r = 1, K = 10))
> out2  <- ode(y = c(y = 12), times, derivs, parms = c(r = 1, K = 10))
> plot(out, out2, lwd = 2)
```



Plotting multiple scenarios . . .

. . . with many or an unknown number of outputs in a list

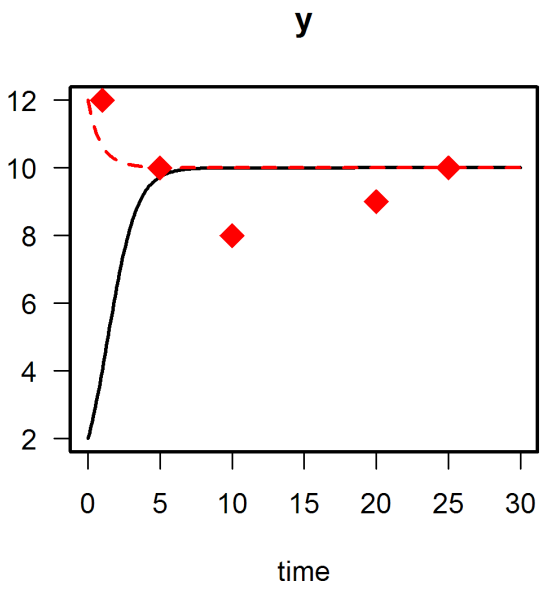
```
> outlist <- list()
> plist <- cbind(r = runif(30, min = 0.1, max = 5),
+                K = runif(30, min = 8,   max = 15))
> for (i in 1:nrow(plist))
+   outlist[[i]] <- ode(y = c(y = 2), times, derivs, parms = plist[i,])
> plot(out, outlist)
```



Observed data

Arguments obs and obspar are used to add observed data

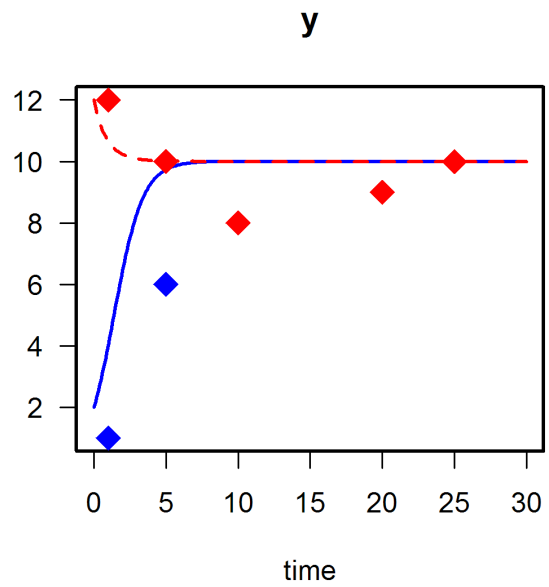
```
> obs2 <- data.frame(time = c(1, 5, 10, 20, 25),
+                    y = c(12, 10, 8, 9, 10))
> plot(out, out2, obs = obs2,
+   obspar = list(col = "red", pch = 18, cex = 2))
```



Observed data

A list of observed data is allowed

```
> obs2 <- data.frame(time = c(1,5,10,20,25), y = c(12,10,8,9,10))
> obs1 <- data.frame(time = c(1,5,10,20,25), y = c(1,6,8,9,10))
> plot(out, out2, col = c("blue", "red"), lwd = 2,
+      obs = list(obs1, obs2),
+      obspar = list(col = c("blue", "red"), pch = 18, cex = 2))
```



Fitting models to data

Fitting models

Given:

- a dynamic model
- data for one or more state variables

Wanted:

- a set of parameters that fits the data

Approach → package FME:

1. try an initial guess for the parameters
2. define cost function (e.g. least squares) with `modCost()`
3. fit the model with `modFit`
4. plot model and data

Interactive web version of this chapter at:
`examples/FME/fit_twocomp.svg`

Pharmacokinetic two compartment model

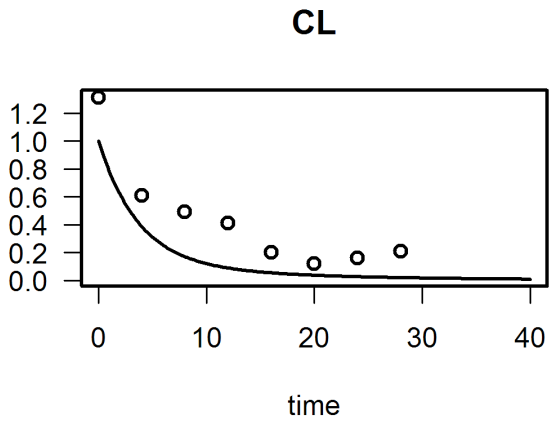
- a substance accumulated in the fat and eliminated by the liver
- two state variables, concentration in the fat C_F and in the liver C_L
- 3 parameters: transport (k_{FL}, k_{LF}) and elimination (k_e)

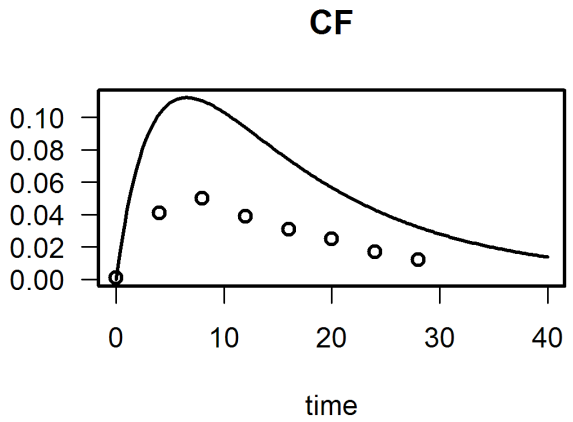
$$\frac{dC_L}{dt} = k_{FL} C_F - k_{LF} C_L - k_e C_L$$
$$\frac{dC_F}{dt} = k_{LF} C_L - k_{FL} C_F$$

```
> library("FME")
> twocomp <- function (time, y, parms, ...) {
+   with(as.list(c(parms, y)), {
+     dCL <- kFL * CF - kLF * CL - ke * CL  # concentration in liver
+     dCF <-    kLF * CL  - kFL * CF        # concentration in fat
+     list(c(dCL, dCF))
+   })
+ }
```

Data and initial guess

```
> dat <- data.frame(
+   time = seq(0, 28, 4),
+   CL = c(1.31,  0.61,  0.49, 0.41,  0.20,  0.12,  0.16,  0.21),
+   CF = c(1e-03, 0.041, 0.05, 0.039, 0.031, 0.025, 0.017, 0.012)
+ )
> parms <- c(ke = 0.2, kFL = 0.1, kLF = 0.05)
> times <- seq(0, 40, length=200)
> y0      <-  c(CL = 1, CF = 0)
> out1 <- ode(y0, times, twocomp, parms)
> plot(out1, obs = dat)
```





Define cost function (least squares):

```
> cost <- function(p) {
+   out  <-  ode(y0, times, twocomp, p)
+   modCost(out, dat, weight = "none") # try weight = "std" or "mean"
+ }
```

Note:

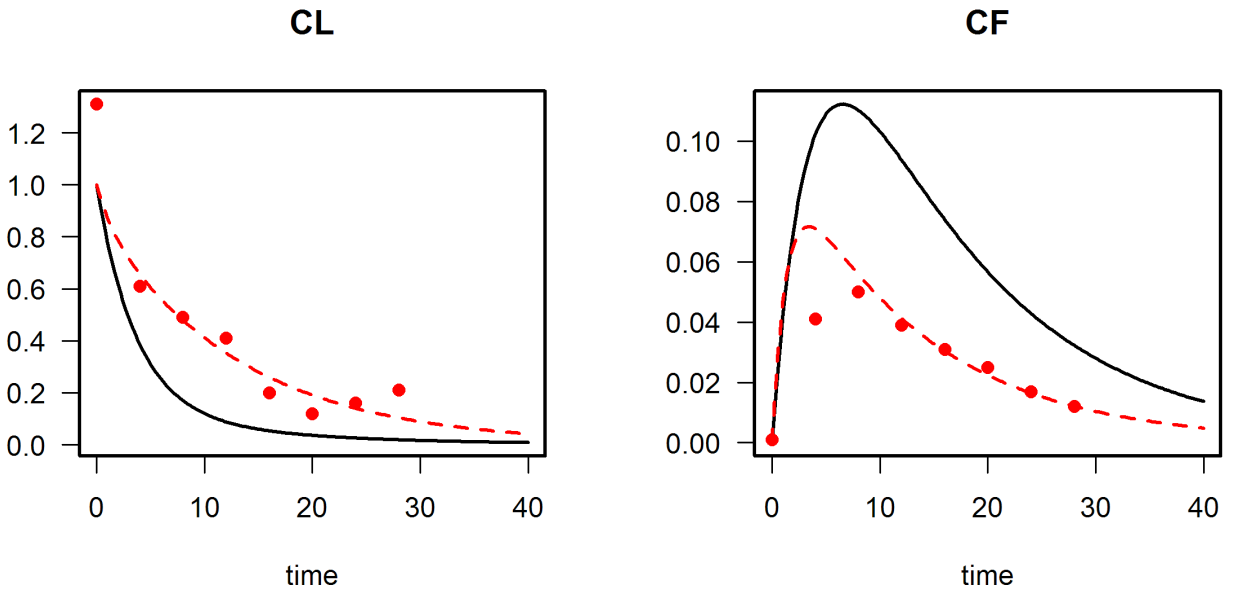
- naming of oservation and simulation data must be identical
- data may be given in cross table (wide) or data base format (long)
- different scaling and weighting options
- optional: sequential build-up of cost function

Fit the model:

```
> parms <- c(ke = 0.2, kFL = 0.1, kLF = 0.05)
> fit <- modFit(f = cost, p = parms)
> summary(fit)

Parameters:
    Estimate Std. Error t value Pr(>|t|)
ke   0.08546    0.01256   6.803 1.26e-05 ***
kFL  0.67293    4.66953   0.144    0.888
kLF  0.06970    0.49269   0.141    0.890
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.09723 on 13 degrees of freedom

Parameter correlation:
        ke    kFL    kLF
ke  1.0000 0.4643 0.4554
kFL 0.4643 1.0000 0.9932
kLF 0.4554 0.9932 1.0000
```

Compare output with data

```
> out1 <- ode(y0, times, twocomp, parms)
> out2 <- ode(y0, times, twocomp, coef(fit))
> plot(out1, out2, obs=dat, obspar=list(pch=16, col="red"))
```



Fit parameters **and initial values**

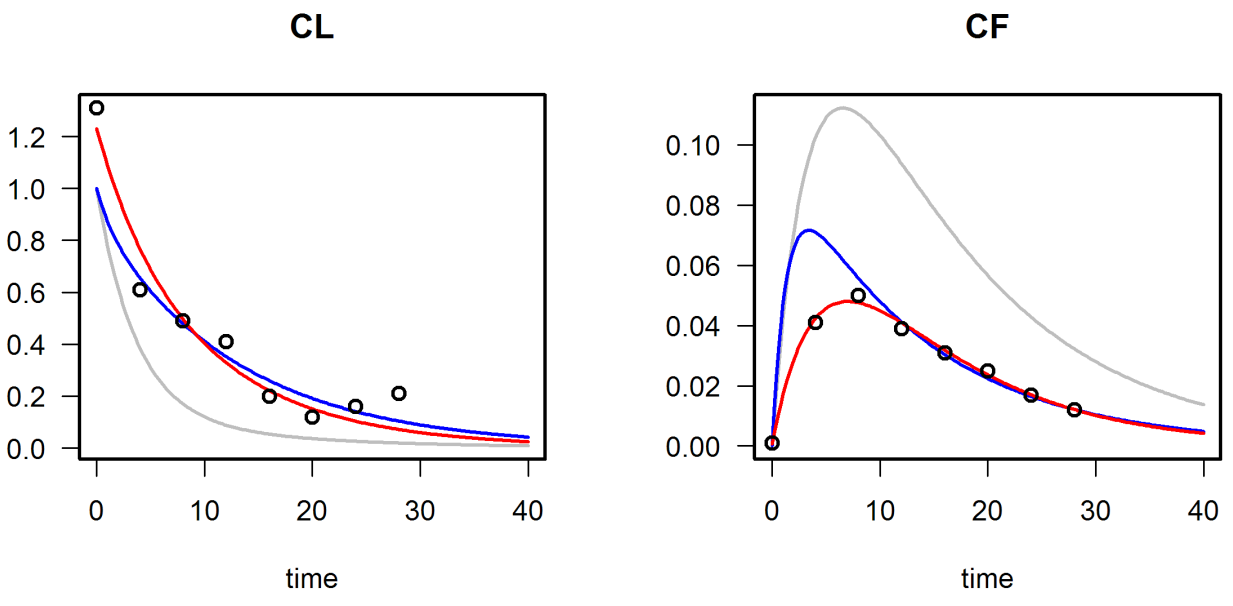
```
> cost <- function(p, data, ...) {
+   yy <- p[c("CL", "CF")]
+   pp <-  p[c("ke", "kFL", "kLF")]
+   out  <-  ode(yy, times, twocomp, pp)
+   modCost(out, data, ...)
+ }
```

Good start parameters can be very important:

```
> #parms <- c(CL = 1.2, CF = 0.0,   ke = 0.2, kFL = 0.1, kLF = 0.05)
> parms  <- c(CL = 1.2, CF = 0.001, ke = 0.2, kFL = 0.1, kLF = 0.05)
> fit <- modFit(f = cost, p = parms, data = dat, weight = "std",
+         lower = rep(0, 5), upper = c(2,2,1,1,1), method = "Marq")
```

Fit parameters and initial values

```
> y0 <- coef(fit)[c("CL", "CF")]
> pp <- coef(fit)[c("ke", "kFL", "kLF")]
> out3 <- ode(y0, times, twocomp, pp)
> plot(out1, out2, out3, obs=dat, col=c("grey", "blue", "red"), lty = 1
```



```
> summary(fit)

Parameters:
     Estimate Std. Error t value Pr(>|t|)
CL  1.2301401  0.0721462  17.051 2.94e-09 ***
CF  0.0006832  0.0033118   0.206     0.84
ke  0.1073351  0.0113231   9.479 1.26e-06 ***
kFL 0.1770353  0.0289383   6.118 7.55e-05 ***
kLF 0.0153855  0.0020288   7.584 1.08e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.2032 on 11 degrees of freedom

Parameter correlation:
           CL         CF       ke     kFL     kLF
CL   1.000000  0.003156  0.54175 -0.3837 -0.5494
CF   0.003156  1.000000  0.04449 -0.2229 -0.3529
ke   0.541754  0.044491  1.00000 -0.7083 -0.4287
kFL -0.383687 -0.222896 -0.70829  1.0000  0.8339
kLF -0.549369 -0.352909 -0.42872  0.8339  1.0000
```

Steady-state

Solver overview, 1-D, 2-D, 3-D

Two packages for Steady-state solutions:

ReacTran: methods for numerical approximation of PDEs

- tran.1D(C, C.up, C.down, D, v, ...)
- tran.2D, tran.3D

rootSolve: special solvers for roots

- `steady` for 0-D models
- `steady.1D`, `steady.2D`, `steady.3D` for 1-D, 2-D, 3-D models

[18] Soetaert, K. and Meysman, F. (2012) Reactive transport in aquatic ecosystems: Rapid model prototyping in the open source software R Environmental Modelling and Software 32, 49–60

[21] Soetaert, K., Petzoldt, T. and Setzer, R. W. (2010 Solving Differential Equations in R The R Journal, 2010, 2, 5-15

Steady-state Solver overview: package rootSolve

Simple problems can be solved iteratively

Function	Description
`stode`	steady-state ODEs by Newton-Raphson method, full or banded Jacobian
`stodes`	steady-state ODEs by Newton-Raphson method, arbitrary sparse Jacobian

Others are solved by dynamically running to steady-state

- `steady( ... method = "runsteady")` for 0-D models
- `steady.1D( ... method = "runsteady")` for 1-D models
- no special solver for higher dimensions - but use `ode.2D`, `ode.3D` from `deSolve` for sufficiently long time

(adapted from [21])

Options of solver functions

Top level function

```
> steady(y, time = NULL, func, parms, method = "stode", ...)
```

Workhorse function: the individual solver

```
> stode(y, time = 0, func, parms = NULL, rtol = 1e-06, atol = 1e-08,
+       ctol = 1e-08, jacfunc = NULL, jactype = "fullint", verbose = FALSE,
+       bandup = 1, banddown = 1, positive = FALSE, maxiter = 100,
+       ynames = TRUE, dllname = NULL, initfunc = dllname, initpar = parms,
+       rpar = NULL, ipar = NULL, nout = 0, outnames = NULL, forcings = NULL,
+       initforc = NULL, fcontrol = NULL, ...)
```

Notes

- `positive = TRUE` forces to find relevant solutions for quantitities that can not be negative.
- `ynames` can be used to label the output – useful for plotting

1-D problem: polluted estuary

Problem formulation

Ammonia and oxygen are described in an estuary. They react to form nitrate. The concentrations are at steady state.

$$\begin{aligned} 0 &= \frac{\partial}{\partial x}\left(D\frac{\partial NH_3}{\partial x}\right) - v\frac{\partial NH_3}{\partial x} - r_{nit} \\ 0 &= \frac{\partial}{\partial x}\left(D\frac{\partial O_2}{\partial x}\right) - v\frac{\partial O_2}{\partial x} - 2r_{nit} + p\cdot(O_2 s - O_2) \\ r_{nit} &= r\cdot NH_3\cdot\frac{O_2}{O_2+k} \end{aligned}$$

- parameters: $k = 1, r = 0.1, p = 0.1, O_2 s = 300, v = 1000, D = 1e^7$
- The estuary is 100 km long.
- The boundary conditions are:

$$NH_3(0) = 500, O_2(0) = 50, NH_3(1e^5) = 10, O_2(1e^5) = 30$$

Polluted estuary in R

define grid:

```
> require(ReacTran)
> N    <- 1000
> Grid <- setup.grid.1D(N = N, L = 100000)
```

derivative function:

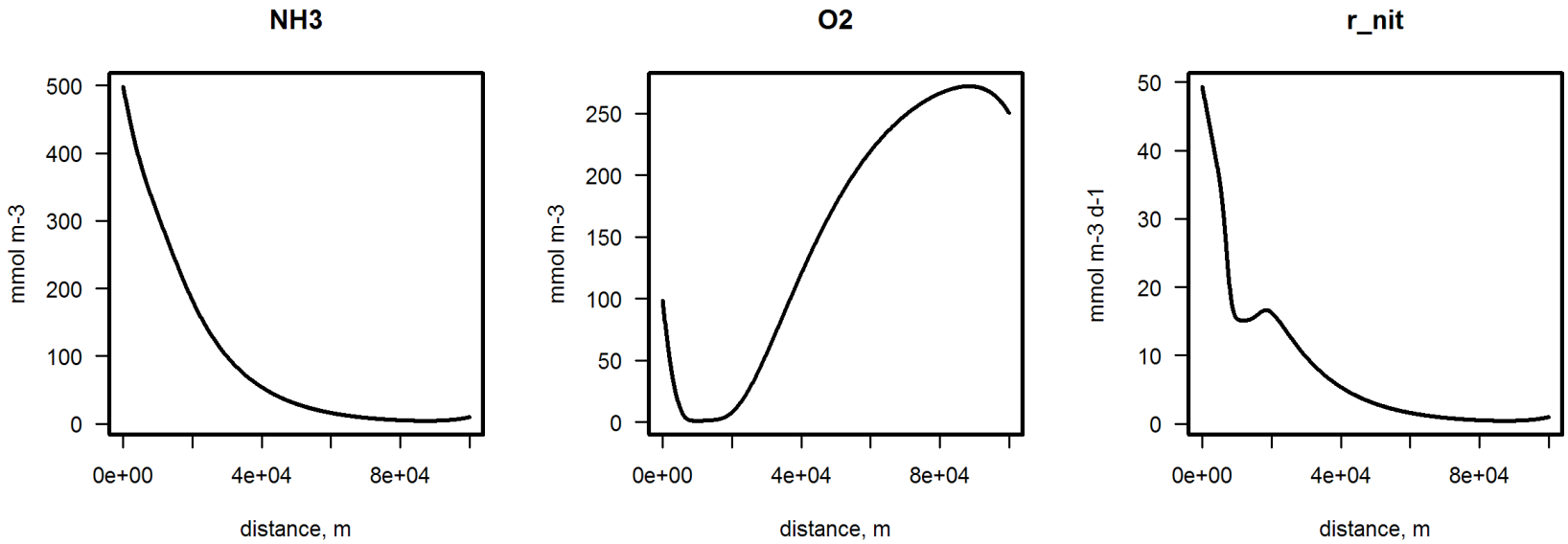
```
> Estuary <- function(t, y, parms)  {
+    NH3 <- y[1:N]
+    O2  <- y[(N+1):(2*N)]
+    tranNH3<- tran.1D (C = NH3, D = 1e7, v = 1000,
+              C.up = 500, C.down = 10,  dx = Grid)$dC
+    tranO2 <- tran.1D (C = O2 , D = 1e7, v = 1000,
+              C.up = 100, C.down = 250, dx = Grid)$dC
+
+    r_nit      <- 0.1 * O2 / (O2 + 1) * NH3
+    dNH3    <- tranNH3 - r_nit
+    dO2     <- tranO2  - 2 * r_nit + 0.1 * (300 - O2)
+    list(c(  dNH3, dO2 ), r_nit = r_nit)
+ }
```

numerical solution:

```
> print(system.time(
+ std <- steady.1D(y = runif(2 * N), parms = NULL, names=c("NH3", "O2"),
+              func = Estuary, dimens = N, positive = TRUE)   ))

   user  system elapsed
   0.11    0.00    0.11
```

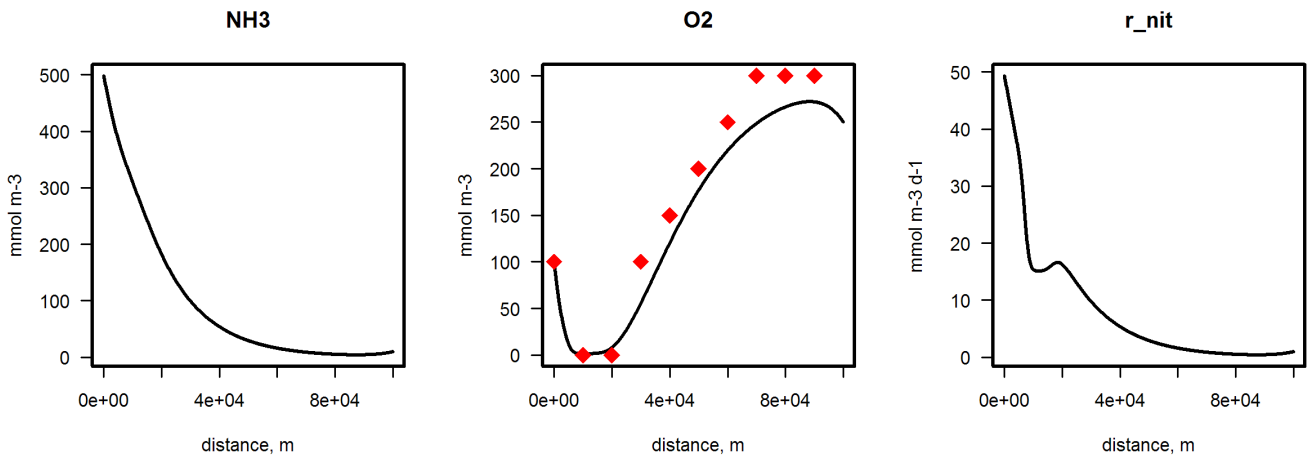
Plotting

```
> plot(std, which = c("NH3", "O2", "r_nit"), lwd = 2,
+      mfrow = c(1,3), grid = Grid$x.mid, xlab = "distance, m",
+      ylab = c("mmol m-3", "mmol m-3", "mmol m-3 d-1"))
```



Plotting with Observations

```
> obs <- data.frame(x = seq(0, 9e4, by = 1e4),
+                   O2 = c(100, 0, 0, 100, 150, 200, 250, 300, 300, 300))
> plot(std, which = c("NH3", "O2", "r_nit"), lwd = 2,
+      obs = obs, obspar = list(pch = 18, col = "red", cex = 2),
+      grid = Grid$x.mid, xlab = "distance, m",
+      ylab = c("mmol m-3", "mmol m-3", "mmol m-3 d-1"), mfrow=c(1,3))
```



Steady-state of a 2-D PDE

Problem formulation

A relatively stiff PDE is the combustion problem, describing diffusion and reaction in a 2-dimensional domain (from [6]). The steady-state problem is:

$$0 = -\nabla \cdot (-K \nabla U) + \frac{R}{\alpha\delta}(1 + \alpha - U) \exp(\delta(1 - 1/U))$$

- The domain is rectangular ([0,1]*[0,1])
- $K = 1, \alpha = 1$, $\delta = 20$, $R = 5$,
- Downstream boundary is prescribed as a known value (1)
- Upstream boundary: zero-flux

2-D combustion problem in R

grid and parameters:

```
> library(ReacTran)
> N  <- 100
> Grid <- setup.grid.1D(0, 1, N = N)
> alfa <- 1; delta <- 20; R <- 5
```

derivative function:

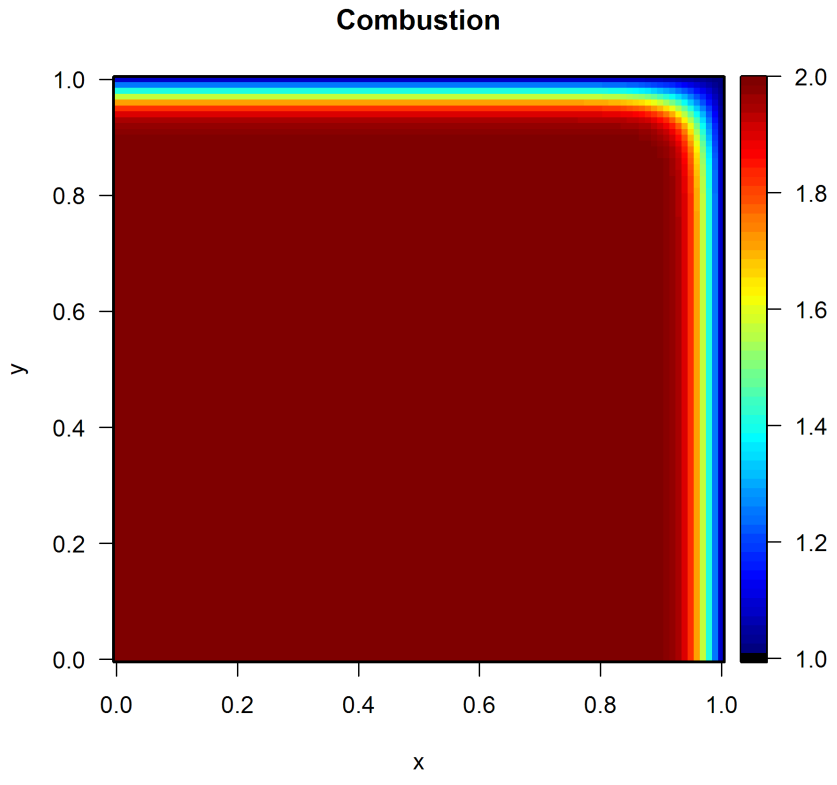
```
> Combustion <- function(t, y, p) {
+    U    <- matrix(nrow = N, ncol = N, data = y)
+
+    reac <- R /alfa/delta * (1+alfa-U) * exp(delta*(1-1/U))
+    tran <- tran.2D(C = U, D.x = 1, flux.x.up = 0, flux.y.up = 0, C.x.down = 1,
+                    C.y.down = 1, dx = Grid, dy = Grid)
+    list (tran$dC+ reac)
+ }
```

solution (10000 equations):

```
> print(system.time(
+ std <- steady.2D(y = rep(1, N*N), parms = NULL, func = Combustion, nspec = 1,
+                   dimens = c(N, N), lrw = 1e6, positive = TRUE)
+ ))

   user  system elapsed
   3.20    0.04    3.29
```

Plotting

```
> image(std, main = "Combustion", legend = TRUE)
```



Steady-state of a 3-D PDE

Problem formulation

3-D problems are computationally heavy - only smaller problems can be solved in R

Model of diffusion and simple reaction in a 3-dimensional domain.

$$0 = -\nabla \cdot (-D\nabla Y) - r * Y$$

- The domain is rectangular ($[0,1] * [0,1] * [0,1]$)
- $D = 1$, $r = 0.025$,
- Initial condition: constant: $U(x, y, 0) = 1$.
- Upstream and Downstream boundaries: $= 1$

3-D problem in R

grid and parameters:

```
> library(ReacTran)
> n   <- 20
> Grid <- setup.grid.1D(0, 1, N = n)
```

derivative function:

```
> diffusion3D <- function(t, Y, par) {
+
+   yy    <- array(dim = c(n, n, n), data = Y)  # vector to 3-D array
+   dY    <- -0.025 * yy                        # consumption
+   BND   <- matrix(nrow = n, ncol = n, 1)      # boundary concentration
+
+   dY <- dY + tran.3D(C = yy,
+       C.x.up = BND, C.y.up = BND, C.z.up = BND,
+       C.x.down = BND, C.y.down = BND, C.z.down = BND,
+       D.x = 1, D.y = 1, D.z = 1,
+       dx = Grid, dy = Grid, dz = Grid)$dC
+   return(list(dY))
+ }
```

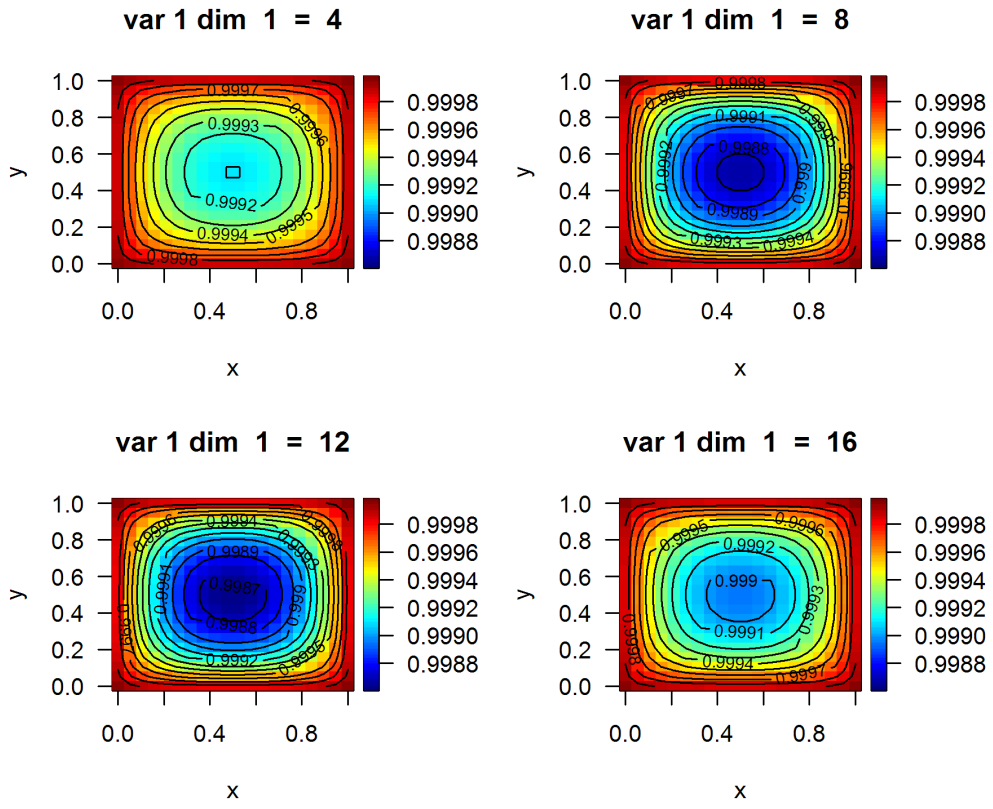
solution (10000 equations):

```
> print(system.time(
+   ST3 <- steady.3D(y = rep(1, n*n*n), func = diffusion3D, parms = NULL,
+                    pos = TRUE, dimens = c(n, n, n), lrw = 2000000)  ))

   user  system elapsed
   2.95    0.02    3.22
```

Plotting

a selection of 2-D projections, in the x-direction

```
> image(ST3, mfrow = c(2, 2), add.contour = TRUE, legend = TRUE,
+       dimselect = list(x = c(4, 8, 12, 16)))
```



Under control: Forcing functions and events

Discontinuities in dynamic models

Most solvers assume that dynamics is *smooth*
However, there can be several types of discontinuities:

- Non-smooth *external variables*
- Discontinuities in the *derivatives*
- Discontinuites in the *values of the state variables*

A solver does not have large problems with first two types of discontinuities, but changing the values of state variables is much more difficult.

External variables in dynamic models

. . . also called forcing functions

Why external variables?

- Some important phenomena are not explicitly included in a differential equation model, but imposed as a *time series*. (e.g. sunlight, important for plant growth is never "modeled").
- Somehow, during the integration, the model needs to know the value of the external variable at each time step!

External variables in dynamic models

Implementation in R

- R has an ingenious function that is especially suited for this task: function `approxfun`
- It is used in two steps:
  - First an interpolating function is constructed, that contains the data. This is done before solving the differential equation.

    ```
    afun <- approxfun(data)
    ```

  - Within the derivative function, this interpolating function is called to provide the interpolated value at the requested time point (`t`):

    ```
    tvalue <- afun(t)
    ```

`?forcings` will open a help file

Example: Predator-Prey model with time-varying input

This example is from [16]

Create an artificial time-series

```
> times <- seq(0, 100, by = 0.1)
> signal <- as.data.frame(list(times = times, import = rep(0, length(times))))
> signal$import <- ifelse((trunc(signal$times) %% 2 == 0), 0, 1)

> signal[8:12,]

   times import
8    0.7      0
9    0.8      0
10   0.9      0
11   1.0      1
12   1.1      1
```

Create the interpolating function, using approxfun

```
> input <- approxfun(signal, rule = 2)

> input(seq(from = 0.98, to = 1.01, by = 0.005))

[1] 0.80 0.85 0.90 0.95 1.00 1.00 1.00
```

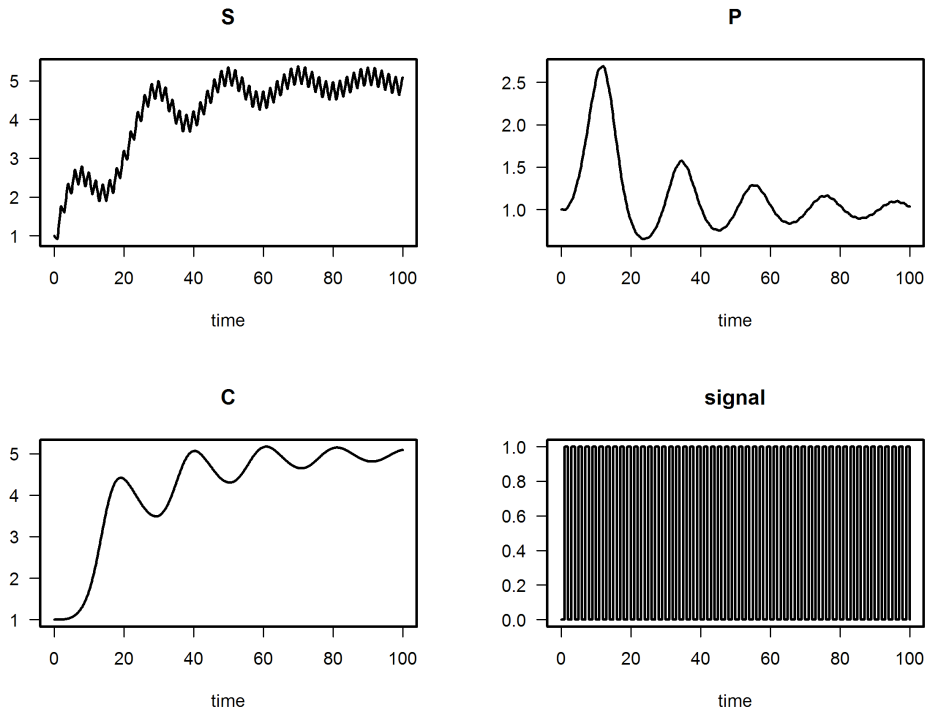
A Predator-Prey model with time-varying input

Use interpolation function in ODE function

```
> SPCmod <- function(t, x, parms) {
+    with(as.list(c(parms, x)), {
+
+    import <- input(t)
+
+    dS <- import - b * S * P + g * C
+    dP <- c * S * P - d * C * P
+    dC <- e * P * C - f * C
+    res <- c(dS, dP, dC)
+    list(res, signal = import)
+  })
+ }

> parms <- c(b = 0.1, c = 0.1, d = 0.1, e = 0.1, f = 0.1, g = 0)
> xstart <- c(S = 1, P = 1, C = 1)
> out <- ode(y = xstart, times = times,  func = SPCmod, parms)
```

Plotting model output

```
> plot(out)
```



Discontinuities in dynamic models: Events

What?

- An event is when the values of state variables change abruptly.

Events in Most Programming Environments

- When an event occurs, the simulation needs to be restarted.
- Use of loops etc. ...
- Cumbersome, messy code

Events in R

- Events are part of a model; no restart necessary
- Separate dynamics inbetween events from events themselves
- Very neat and efficient!

Discontinuities in dynamic models, Events

Two different types of events in R

- Events occur at *known times*
  - Simple changes can be specified in a `data.frame` with:
    - name of state variable that is affected
    - the time of the event
    - the magnitude of the event
    - event method ("replace", "add", "multiply")
  - More complex events can be specified in an `event function` that returns the changed values of the state variables `function(t, y, parms, ...)`.

- Events occur when certain *conditions* are met
  - Event is triggered by a `root` function
  - Event is specified in an `event function`

`?events` will open a help file

A patient injects drugs in the blood

Problem Formulation

- Describe the concentration of the drug in the blood
- Drug injection occurs at known times $\rightarrow$ `data.frame`

Dynamics inbetween events

- The drug decays with rate `b`
- Initially the drug concentration $= 0$

```
> pharmaco <- function(t, blood, p) {
+   dblood <-  - b * blood
+   list(dblood)
+ }

> b    <- 0.6
> yini <- c(blood = 0)
```

A patient injects drugs in the blood

Specifying the event

- Daily doses, at same time of day
- Injection makes the concentration in the blood increase by 40 units.
- The drug injections are specified in a special event `data.frame`

```
> injectevents <- data.frame(var = "blood",
+                            time =  0:20,
+                            value = 40,
+                            method = "add")

> head(injectevents)

    var time value method
1 blood    0    40    add
2 blood    1    40    add
3 blood    2    40    add
4 blood    3    40    add
5 blood    4    40    add
6 blood    5    40    add
```

A patient injects drugs in the blood

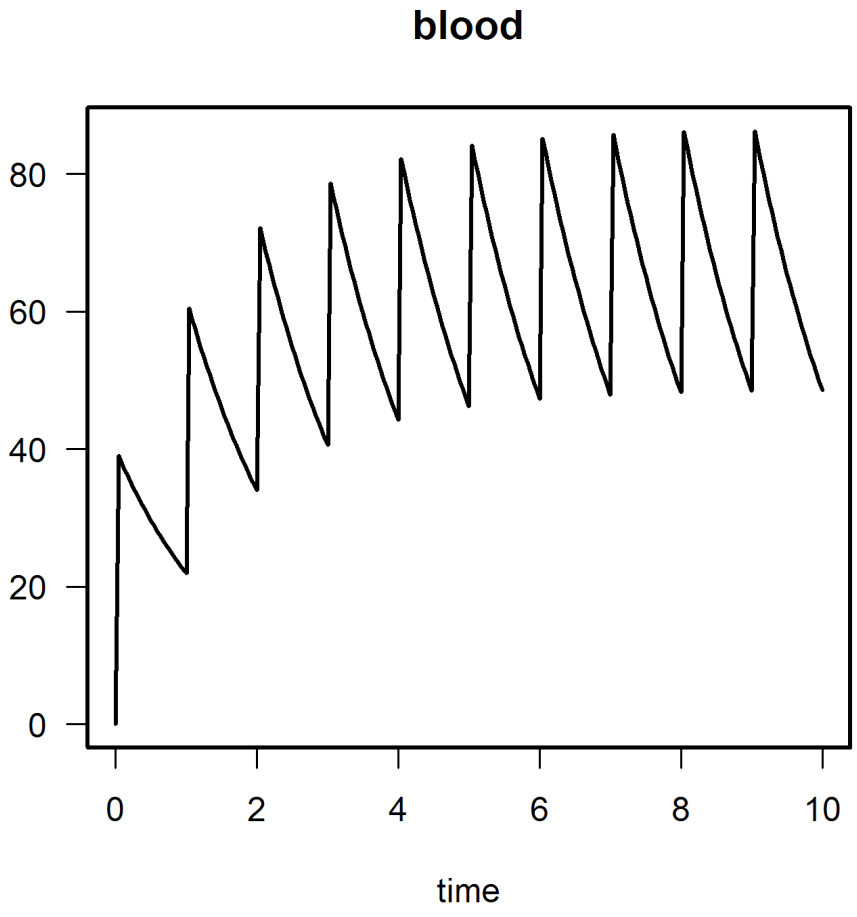
Solve model

- Pass events to the solver in a list
- All solvers in `deSolve` can handle events
- Here we use the "implicit Adams" method

```
> times <- seq(from = 0, to = 10, by = 1/24)
> outDrug <- ode(func = pharmaco, times = times, y = yini,
+             parms = NULL, method = "impAdams",
+             events = list(data = injectevents))
```

plotting model output

```
> plot(outDrug)
```



An event triggered by a root: A Bouncing Ball

Problem formulation

- A ball is thrown vertically from the ground ($y(0) = 0$)
- Initial velocity (y') = 10 $m\ s^{-1}$; acceleration $g = 9.8\ m\ s^{-2}$
- When ball hits the ground, it bounces.

ODEs describe height of the ball above the ground (y)

Specified as 2^{nd} order ODE

$$\begin{aligned} y'' &= -g \\ y(0) &= 0 \\ y'(0) &= 10 \end{aligned}$$

Specified as 1^{st} order ODE

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= -g \\ y_1(0) &= 0 \\ y_2(0) &= 10 \end{aligned}$$

[14] Shampine, L. F.; Gladwell, I. and Thompson, S. (2003) Solving ODEs with MATLAB. Cambridge University Press, 2003, 263

A Bouncing Ball

Dynamics inbetween events

```
> library(deSolve)

> ball <- function(t, y, parms) {
+   dy1 <- y[2]
+   dy2 <- -9.8
+
+   list(c(dy1, dy2))
+ }

> yini  <- c(height = 0, velocity = 10)
```

The Ball Hits the Ground and Bounces

Root: the Ball hits the ground

- The ground is where height $= 0$
- Root function is 0 when $y_1 = 0$

```
> rootfunc <- function(t, y, parms) return (y[1])
```

Event: the Ball bounces

- The velocity changes sign (-) and is reduced by 10%
- Event function returns changed values of both state variables

```
> eventfunc <- function(t, y, parms) {
+   y[1] <- 0
+   y[2] <- -0.9*y[2]
+   return(y)
+ }
```

An event triggered by a root: the bouncing ball

Solve model

- Inform solver that event is triggered by root (`root = TRUE`)
- Pass event function to solver
- Pass root function to solver

```
> times <- seq(from = 0, to = 20, by = 0.01)
> out <- ode(times = times, y = yini, func = ball,
+               parms = NULL, rootfun = rootfunc,
+               events = list(func = eventfunc, root = TRUE))
```

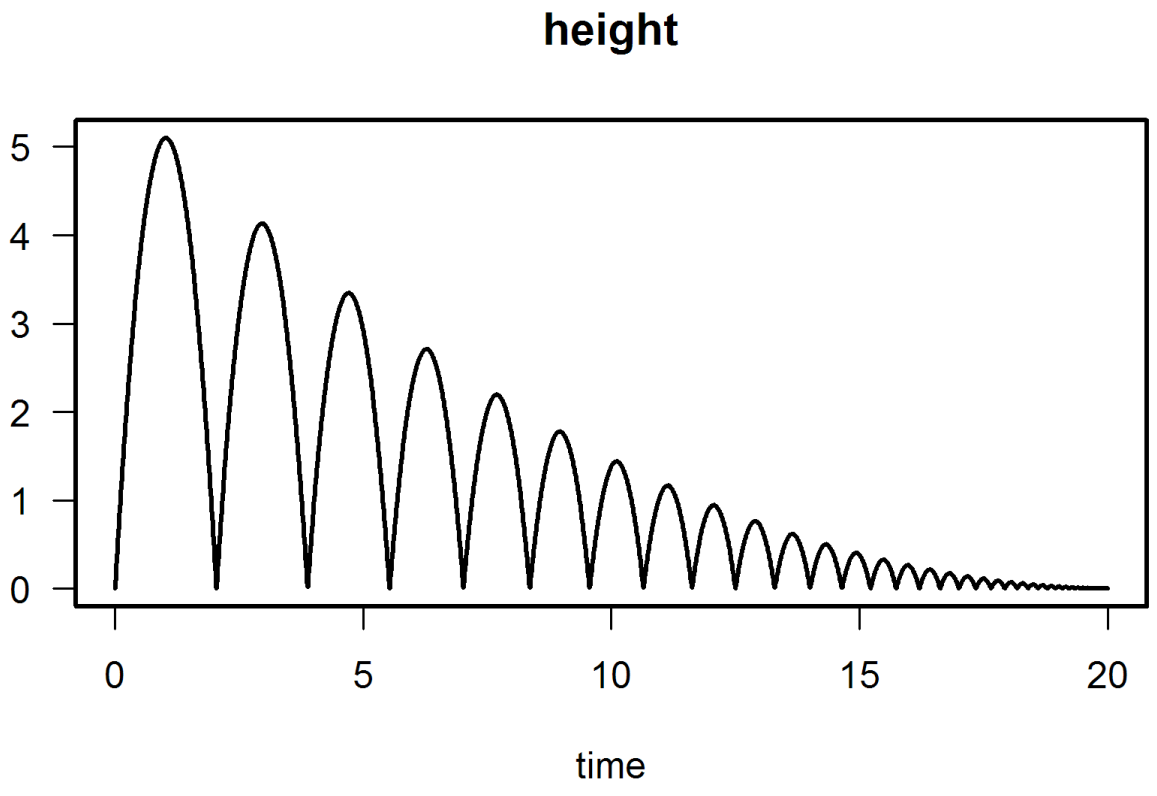
Get information about the root

```
> attributes(out)$troot
```

```
 [1]  2.040816  3.877551  5.530612  7.018367  8.357347  9.562428 10.647001 11.623117
 [9] 12.501621 13.292274 14.003862 14.644290 15.220675 15.739420 16.206290 16.626472
[17] 17.004635 17.344981 17.651291 17.926970 18.175080 18.398378 18.599345 18.780215
[25] 18.942998 19.089501 19.221353 19.340019 19.446817 19.542935 19.629441 19.707294
[33] 19.777362 19.840421 19.897174 19.948250 19.994217
```

An event triggered by a root: the bouncing ball

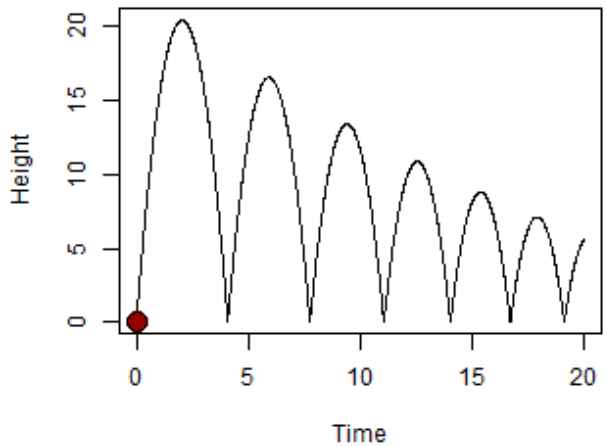
```
> plot(out, select = "height")
```



An event triggered by a root: the bouncing ball

Create Movie-like output

```
for (i in seq(1, 2001, 10)) {
  plot(out, which = "height", type = "l", lwd = 1,
       main = "", xlab = "Time", ylab = "Height"
  )
  points(t(out[i,1:2]), pch = 21, lwd = 1, col = 1, cex = 2,
         bg = rainbow(30, v = 0.6)[20-abs(out[i,3])+1])
  Sys.sleep(0.01)
}
```



Exercise: Add events to a logistic equation

ODE: Logistic growth of a population

$$y' = r \cdot y \cdot \left(1 - \frac{y}{K}\right)$$

$$r = 1, K = 10, y_0 = 2$$

Events: Population harvested according to several strategies

1. No harvesting
2. Every 2 days the population's density is reduced to 50%
3. When the population approaches 80% of its carrying capacity, its density is halved.

Exercise: Add events to a logistic equation - ctd

Tasks:

- Run the model for 20 days
- Implement first strategy in a `data.frame`
- Second strategy requires root and event function
- Use file `examples/logisticEvent.R.txt` as a template

Delay Differential Equations

What?

Delay Differential Equations are similar to ODEs except that they involve *past* values of variables and/or derivatives.

DDEs in R: R-package deSolve

- `dede` solves DDEs
- `lagvalue` provides lagged values of the state variables
- `lagderiv` provides lagged values of the derivatives

Example: Chaotic Production of White Blood Cells

Mackey-Glass Equation:

- y: current density of white blood cells,
- y_τ is the density τ time-units in the past,
- first term equation is production rate
- b is destruction rate

$$\begin{aligned} y' &= a y_\tau \frac{1}{1+y_\tau^c} - by \\ y_\tau &= y(t-\tau) \\ y_t &= 0.5 \qquad \text{for } t \le 0 \end{aligned} \tag{1}$$

- For $\tau = 10$ the output is periodic,
- For $\tau = 20$ cell densities display a chaotic pattern

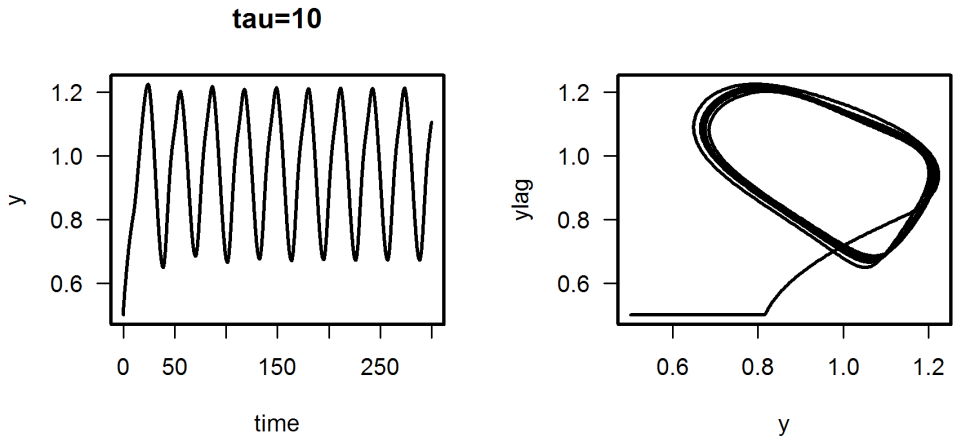
[9] Mackey, M. C. and Glass, L. (1977) Oscillation and chaos in physiological control systems. Science 197, 287–289

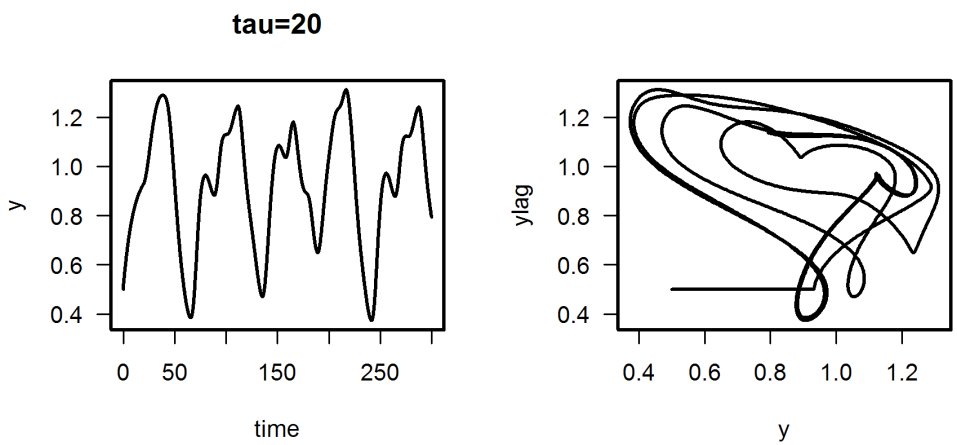
Solution in R

```
> library(deSolve)
> retarded <- function(t, y, parms, tau) {
+   tlag <- t - tau
+   if (tlag <= 0)
+     ylag <- 0.5
+   else
+     ylag <- lagvalue(tlag)
+
+   dy <- 0.2 * ylag * 1/(1+ylag^10) - 0.1 * y
+   list(dy = dy, ylag = ylag)
+ }
> yinit <- 0.5
> times <- seq(from = 0, to = 300, by = 0.1)
> yout1 <- dede(y = yinit, times = times, func = retarded, parms = NULL, tau = 10)
> yout2 <- dede(y = yinit, times = times, func = retarded, parms = NULL, tau = 20)
```

Solution in R

```
> plot(yout1, lwd = 2, main = "tau=10", ylab = "y", mfrow = c(2, 2), which = 1)
> plot(yout1[,-1], type = "l", lwd = 2, xlab = "y")
> plot(yout2, lwd = 2, main = "tau=20", ylab = "y", mfrow = NULL, which = 1)
> plot(yout2[,-1], type = "l", lwd = 2, xlab = "y")
```





Exercise: the Lemming model

A nice variant of the logistic model is the DDE lemming model:

$$y' = r \cdot y(1 - \frac{y(t-\tau)}{K}) \tag{2}$$

Use file `examples/ddelemming.R.txt` as a template to implement this model

- initial condition $y(t = 0) = 19.001$
- parameter values $r = 3.5$, $\tau = 0.74$, $K = 19$
- history $y(t) = 19$ for $t < 0$
- Generate output for t in [0, 40].

[15] Shampine, L. and Thompson, S. (2001) Solving DDEs in MATLAB. App. Numer. Math. 37, 441-458

Diffusion, advection and reaction: Partial differential equations (PDE) with ReacTran

Partial Differential Equations

Many second-order PDEs can be written as advection-diffusion problems:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} + f(t, x, C)$$

. . . same for 2-D and 3-D

Example: wave equation in 1-D

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} \tag{3}$$

can be written as:

$$\begin{aligned} \frac{du}{dt} &= v \\ \frac{\partial v}{\partial t} &= c^2\frac{\partial^2 u}{\partial x^2} \end{aligned} \tag{4}$$

Three packages for solving PDEs in R

ReacTran: methods for numerical approximation of PDEs

- tran.1D(C, C.up, C.down, D, v, ...)
- tran.2D, tran.3D

deSolve: general-purpose solvers for time-varying cases

- ode.1D(y, times, func, parms, nspec, dimens, method, names, ...)
- ode.2D, ode.3D

rootSolve: special solvers for time-invariant cases

- steady.1D(y, time, func, parms, nspec, dimens, method, names, ...)
- steady.2D, steady.3D

[18, 22, 17]

Numerical solution of the wave equation

```
library(ReacTran)

wave <- function (t, y, parms) {
  u <- y[1:N]
  v <- y[(N+1):(2*N)]
  du <- v
  dv <- tran.1D(C = u, C.up = 0, C.down = 0, D = 1,
                dx = xgrid)$dC
list(c(du, dv))
}
xgrid <- setup.grid.1D(-100, 100, dx.1 = 0.2)
x     <- xgrid$x.mid
N     <- xgrid$N
uini  <- exp(-0.2*x^2)
vini  <- rep(0, N)
yini  <- c(uini, vini)
times <- seq (from = 0, to = 50, by = 1)

out <- ode.1D(yini, times, wave, parms, method = "adams",
              names = c("u", "v"), dimens = N)

image(out, grid = x)
```

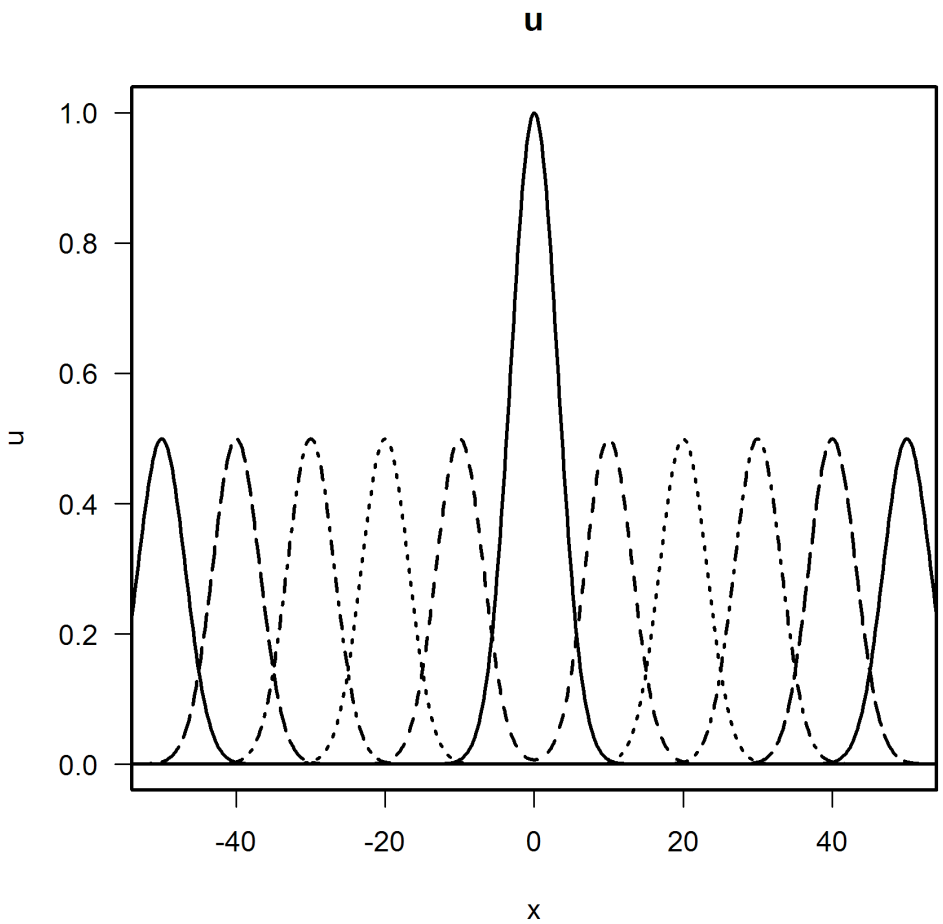
http://desolve.r-forge.r-project.org

Methods from ReacTran

Numerical method provided by the deSolve package

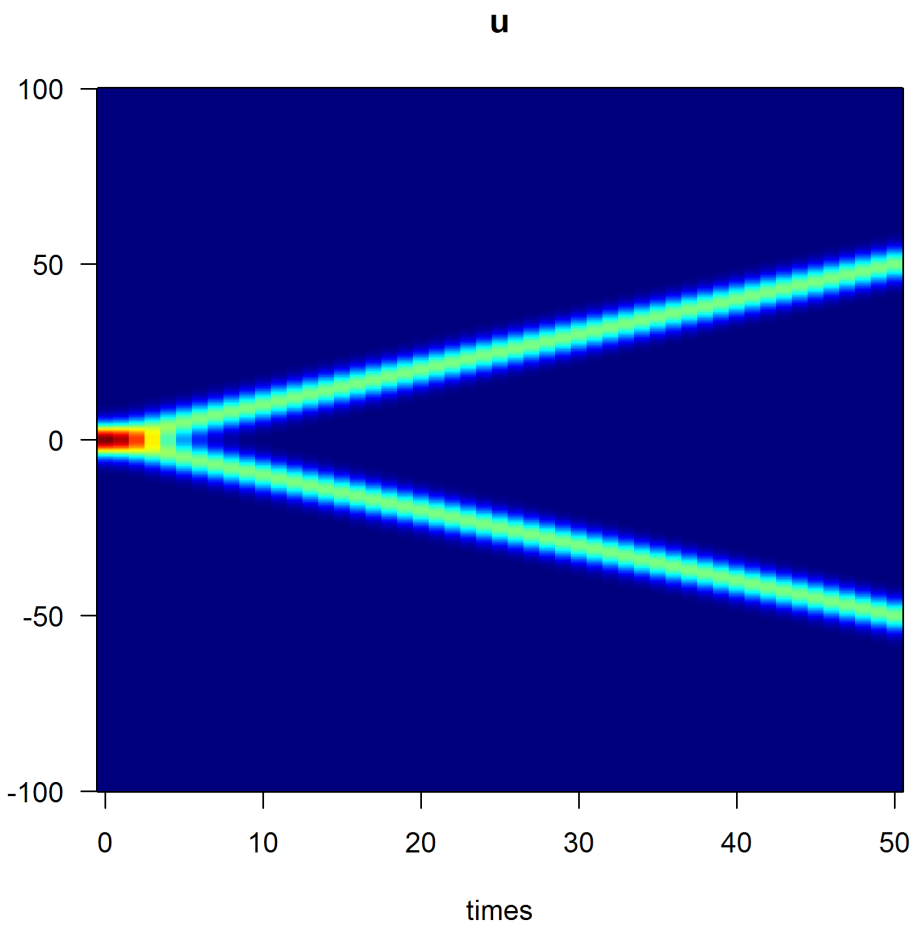
Plotting 1-D PDEs: matplot.1D

```
> outtime <- seq(from = 0, to = 50, by = 10)
> matplot.1D(out, which = "u", subset = time %in% outtime, grid = x,
+     xlab = "x", ylab = "u", type = "l", lwd = 2, xlim = c(-50, 50), col="black")
```



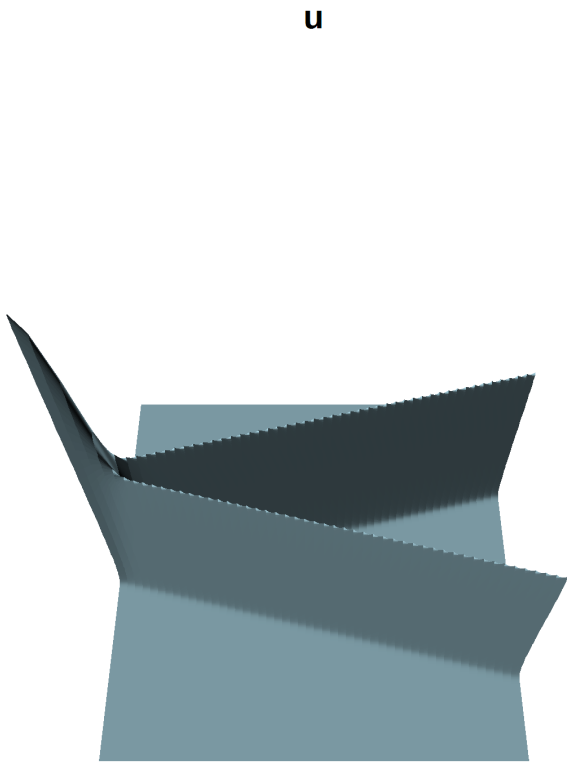
Plotting 1-D PDEs: image

```
> image(out, which = "u", grid = x)
```



Plotting 1-D PDEs: persp plots

```
> image(out, which = "u", grid = x, method = "persp", border = NA,
+       col = "lightblue", box = FALSE, shade = 0.5, theta = 0, phi = 60)
```



Exercise: the Brusselator

Problem formulation

The Brusselator is a model for an auto-catalytic chemical reaction between two products, A and B, and producing also C and D in a number of intermediary steps.

$$\begin{aligned} A &\xrightarrow{k_1} X_1 \\ B + X_1 &\xrightarrow{k_2} X_2 + C \\ 2X_1 + X_2 &\xrightarrow{k_3} 3X_1 \\ X_1 &\xrightarrow{k_4} D \end{aligned}$$

where the k_i are the reaction rates.

[7] Lefever, R., Nicolis, G. and Prigogine, I. (1967) On the occurrence of oscillations around the steady state in systems of chemical reactions far from equilibrium Journal of Chemical Physics 47, 1045–1047

Exercise: Implement the Brusselator in 1-D

$$\frac{\partial X_1}{\partial t} = D_{X_1}\frac{\partial^2 X_1}{\partial x^2} + 1 + X_1^2 X_2 - 4X_1$$

$$\frac{\partial X_2}{\partial t} = D_{X_2}\frac{\partial^2 X_2}{\partial x^2} + 3X_1 - X_1^2 X_2$$

Tasks

- The grid x extends from 0 to 1, and consists of 50 cells.
- Initial conditions:

$$X_1(0) = 1 + sin(2 * \pi * x), X_2(0) = 3$$

- Generate output for $t = 0, 1, \ldots 10$.
- Use file implementing the wave equation as a template: `examples/wave.R.txt`

2-D wave equation: Sine-Gordon

Problem formulation

The Sine-Gordon equation is a non-linear hyperbolic (wave-like) partial differential equation involving the sine of the dependent variable.

$$\frac{\partial^2 u}{\partial t^2} = D\frac{\partial^2 u}{\partial x^2} + D\frac{\partial^2 u}{\partial y^2} - \sin u \tag{5}$$

Rewritten as two first order differential equations:

$$\begin{aligned} \frac{du}{dt} &= v \\ \frac{\partial v}{\partial t} &= D\frac{\partial^2 u}{\partial x^2} + D\frac{\partial^2 u}{\partial y^2} - \sin u \end{aligned} \tag{6}$$

2-D Sine-Gordon in R

grid:

```
> Nx  <- Ny <- 100
> xgrid <- setup.grid.1D(-7, 7, N = Nx); x <- xgrid$x.mid
> ygrid <- setup.grid.1D(-7, 7, N = Ny); y <- ygrid$x.mid
```

derivative function:

```
> sinegordon2D <- function(t, C, parms) {
+    u <- matrix(nrow = Nx, ncol = Ny, data = C[1 : (Nx*Ny)])
+    v <- matrix(nrow = Nx, ncol = Ny, data = C[(Nx*Ny+1) : (2*Nx*Ny)])
+    dv <- tran.2D (C = u, C.x.up = 0, C.x.down = 0, C.y.up = 0, C.y.down = 0,
+                   D.x = 1, D.y = 1, dx = xgrid, dy = ygrid)$dC  -   sin(u)
+    list(c(v, dv))
+ }
```

initial conditions:

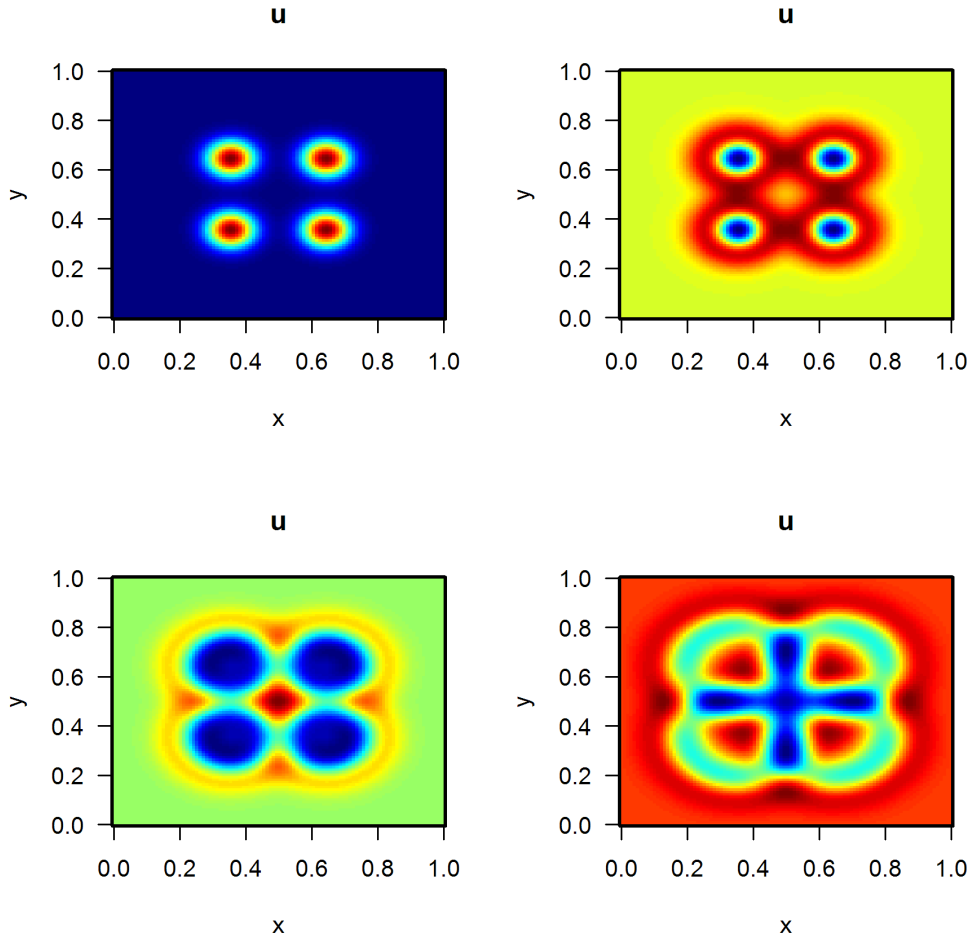
```
> peak <- function (x, y, x0, y0)  return(exp(-( (x-x0)^2 + (y-y0)^2)))
> uini <- outer(x, y, FUN = function(x, y) peak(x, y, 2,2) + peak(x, y,-2,-2)
+                                        + peak(x, y,-2,2) + peak(x, y, 2,-2))
> vini <- rep(0, Nx*Ny)
```

solution:

```
> out  <- ode.2D (y = c(uini,vini), times = 0:3, parms = 0, func = sinegordon2D,
+          names = c("u", "v"), dimens = c(Nx, Ny), method = "ode45")
```

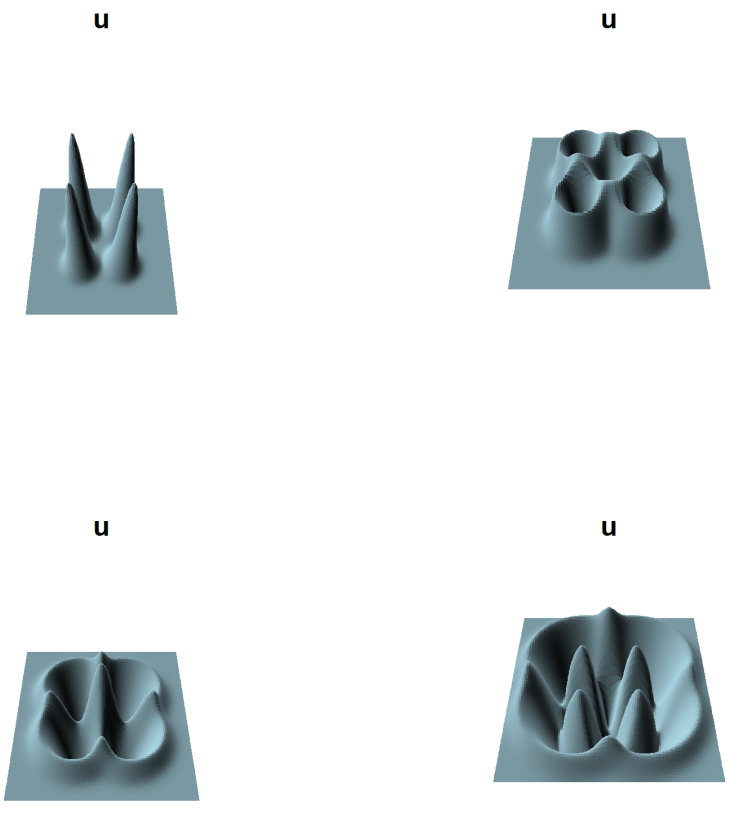
Plotting 2-D PDEs: image plots

```
> image(out, which = "u", grid = list(x, y), mfrow = c(2,2), ask = FALSE)
```



Plotting 2-D PDEs: persp plots

```
> image(out, which = "u", grid = list(x, y), method = "persp", border = NA,
+       col = "lightblue", box = FALSE, shade = 0.5, theta = 0, phi = 60,
+       mfrow = c(2,2), ask = FALSE)
```



Movie-like output of 2-D PDEs

```
out  <- ode.2D (y = c(uini, vini), times = seq(0, 3, by = 0.1),
                parms = NULL, func = sinegordon2D,
                names=c("u", "v"), dimens = c(Nx, Ny),
                method = "ode45")
image(out, which = "u", grid = list(x = x, y = y),
     method = "persp", border = NA,
     theta = 30, phi = 60, box = FALSE, ask = FALSE)
```

Exercise: Implement the Brusselator in 2-D

$$\frac{\partial X_1}{\partial t} = D_{X_1}\frac{\partial^2 X_1}{\partial x^2} + D_{X_1}\frac{\partial^2 X_1}{\partial y^2} + 1 + X_1^2 X_2 - 4X_1$$

$$\frac{\partial X_2}{\partial t} = D_{X_2}\frac{\partial^2 X_1}{\partial x^2} + D_{X_2}\frac{\partial^2 X_1}{\partial y^2} + 3X_1 - X_1^2 X_2$$

Tasks

- The grids x and y extend from 0 to 1, and consist of 50 cells.
- Parameter settings: diffusion coefficient:

$$D_{X_1} = 2; D_{X_2} = 8 * D_{X_1}$$

- Initial condition for X_1, X_2: random numbers inbetween 0 and 1.
- Generate output for t = 0, 1, ... 8
- Use the file implementing the Sine-Gordon equation as a template: `examples/sinegordon.R.txt`

Differential-Algebraic Equations

Solver overview, examples

Two solvers for DAEs in R-package deSolve:

daspk

- a backward differentiation formula (BDF)
- DAEs of index 1 only
- Can solve DAEs in form $My' = f(x, y)$ and $F(x, y, y') = 0$

radau

- an implicit Runge-Kutta formula (BDF)
- DAEs of index ≤ 3
- Can solve DAEs in form $My' = f(x, y)$ only

. . . more in package deTestSet

- . . .

[1] Brenan, K. E., Campbell, S. L. and Petzold, L. R. (1996) Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations. SIAM Classics in Applied Mathematics.
[4] Hairer, E. and Wanner, G. (2010) Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems. Second Revised Edition, Springer-Verlag.

Options of solver functions

```
daspk (y, times, func = NULL, parms, dy, res, mass, ...)
radau (y, times, func, parms, nind, mass, ...)
```

- `func` and `mass`: for $My' = f(x, y)$
- `res`: for $F(x, y, y') = 0$
- `nind`: number of variables of index 1, 2, and 3 $\Rightarrow$ equations should be sorted accordingly
- `radau` does not require specification of (consistent) initial derivatives (`dy`)

Implicit DAE: Robertson problem

Problem formulation

A classic problem to test stiff ODE/DAE solvers, given by Robertson (1966), written as a DAE (of index 1):

$$\begin{aligned} y_1' &= -0.04y_1 + 10^4 y_2 y_3 \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - 3e^7 y_2^2 \\ 1 &= y_1 + y_2 + y_3 \end{aligned} \quad \Rightarrow \quad \begin{aligned} 0 &= -y_1' - 0.04y_1 + 10^4 y_2 y_3 \\ 0 &= -y_2' + 0.04y_1 - 10^4 y_2 y_3 - 3e^7 y_2^2 \\ 0 &= -1 + y_1 + y_2 + y_3 \end{aligned}$$

The third equation is to conserve the total concentration of y_1, y_2, y_3

- initial conditions: $y_1 = 1, y_2 = 0, y_3 = 0$.
- output for $t = 10^{[0,\ 0.1,\ 0.2,\ldots 10]}$
- solve with daspk

[12] Robertson, H. H. (1966) The solution of a set of reaction rate equations. In Walsh, J. (ed.) Numerical Analysis: An Introduction, Academic Press, 178-182

Robertson DAE in R

residual function (4 mandatory arguments):

```
> RobertsonDAE <- function(t, y, dy, parms)  {
+
+   res1 <- -dy[1] - 0.04*y[1] + 1e4*y[2]*y[3]
+   res2 <- -dy[2] + 0.04*y[1] - 1e4*y[2]*y[3] - 3e7* y[2]^2
+   res3 <- - 1 + y[1] + y[2] + y[3]
+
+   list(c(res1, res2, res3))
+ }
```

initial conditions (values, derivatives):

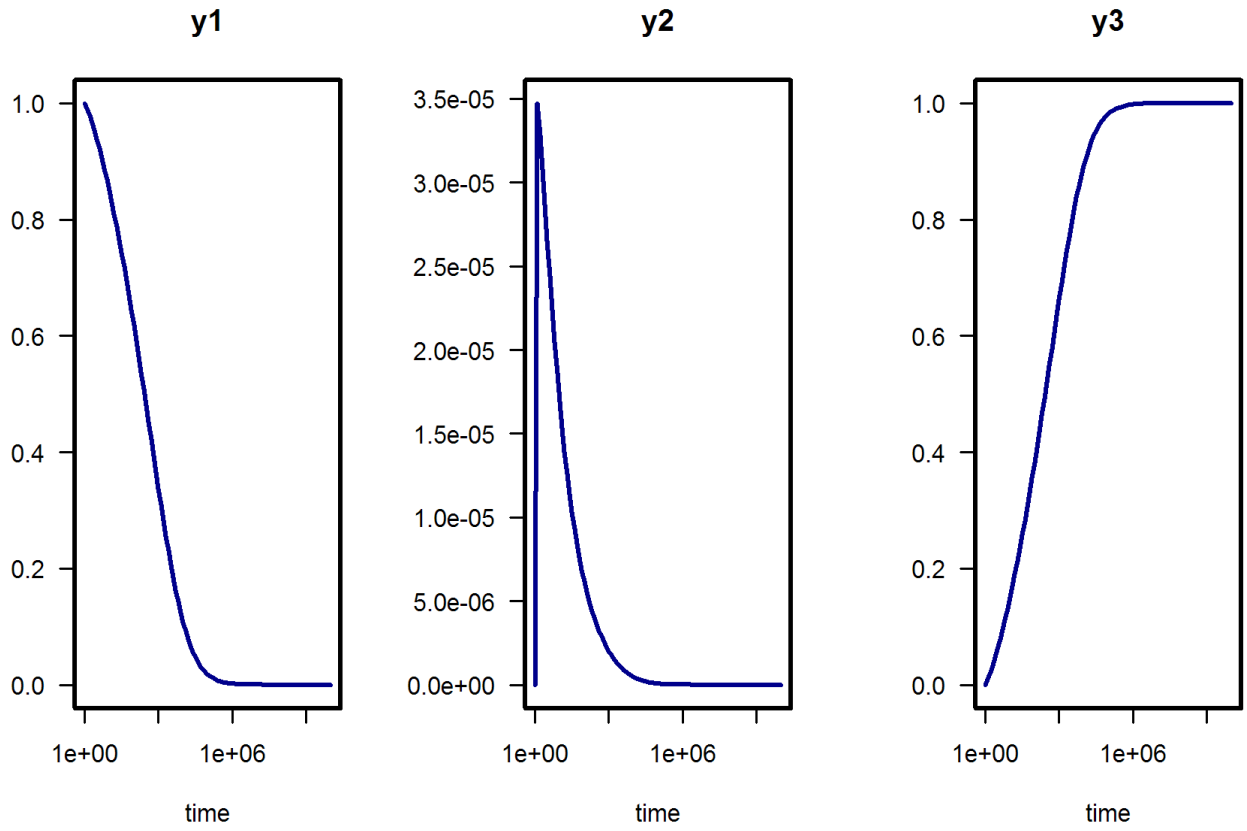
```
> yini  <- c(y1 = 1.0, y2 = 0, y3 = 0)
> dyini <- rep(0, 3)   # rough guess often good enough
```

solution:

```
> times <- 10^(seq(from = 0, to = 10, by = 0.1))
> out <- daspk(y = yini, dy = dyini, res = RobertsonDAE, parms = NULL,
+              times = times)
```

Plotting

```
> plot(out, log = "x", col = "darkblue", lwd = 2, mfrow=c(1,3))
```



The pendulum

Problem formulation, an index 3 DAE

Original equations:

$$\begin{aligned} x' &= u \\ y' &= v \\ u' &= -\lambda x \\ v' &= -\lambda y - g \\ 0 &= x^2 + y^2 - L^2 \end{aligned}$$

$\Rightarrow$

M.y' = f(x,y)

$$\begin{vmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{vmatrix} . \begin{vmatrix} x' \\ y' \\ u' \\ v' \\ \lambda \end{vmatrix} = \begin{vmatrix} u \\ v \\ -\lambda x \\ -\lambda y - g \\ x^2 + y^2 - L^2 \end{vmatrix}$$

- initial conditions: $x = 1, y = 0, u = 0, v = 1, \lambda = 1$
- x and y variables of index 1, u, v of index 2, λ of index 3
- solve in [0,10]

[1, 4]

Pendulum problem in R

derivative function:

```
> pendulum <- function (t, Y, parms) {
+   with (as.list(Y),
+     list(c(u,
+            v,
+            -lam * x,
+            -lam * y - 9.8,
+            x^2 + y^2 -1
+          ))
+   )
+ }
```

mass matrix and index vector:

```
> M <- diag(nrow = 5)
> M[5, 5] <- 0
> index <- c(2, 2, 1)
```

initial conditions:

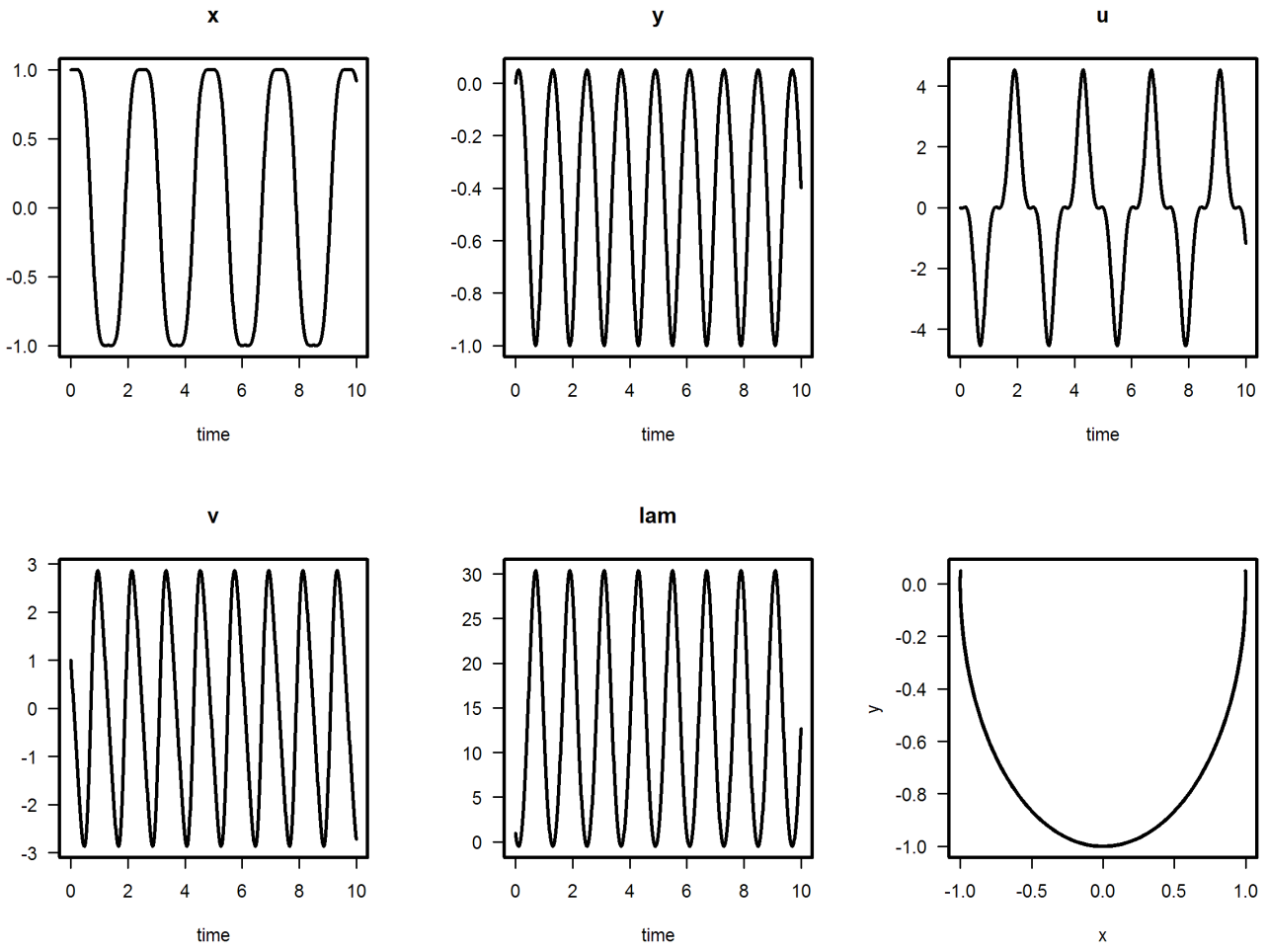
```
> yini <- c(x = 1, y = 0, u = 0, v = 1, lam = 1)
```

solution :

```
> times <- seq(from = 0, to = 10, by = 0.01)
> out <- radau (y = yini, func = pendulum, parms = NULL,
+               times = times, mass = M, nind = index)
```

Plotting

```
> plot(out, type = "l", lwd = 2)
> plot(out[, c("x", "y")], type = "l", lwd = 2)
```



Speeding up: Matrices and compiled code

Methods for speeding up

1. Use matrices,
2. Implement essential parts in compiled code (Fortran, C),
3. Implement the full method in compiled code.

Formulating a model with matrices and vectors can lead to a considerable speed gain – and compact code – while retaining the full flexibility of R. The use of compiled code saves even more CPU time at the cost of a higher development effort.

Use of matrices

A Lotka-Volterra model with 4 species

```
>   model <- function(t, n, parms) {
+     with(as.list(c(n, parms)), {
+       dn1 <- r1 * n1 - a13 * n1 * n3
+       dn2 <- r2 * n2 - a24 * n2 * n4
+       dn3 <- a13 * n1 * n3 - r3 * n3
+       dn4 <- a24 * n2 * n4 - r4 * n4
+     return(list(c(dn1, dn2, dn3, dn4)))
+   })
+ }
> parms <- c(r1 = 0.1, r2 = 0.1, r3 = 0.1, r4 = 0.1, a13 = 0.2, a24 = 0.1)
> times = seq(from = 0, to = 500, by = 0.1)
> n0  = c(n1 = 1, n2 = 1, n3 = 2, n4 = 2)

> system.time(out <- ode(n0, times, model, parms))

   user  system elapsed
   0.62    0.00    0.62
```

Source: examples/lv-plain-or-matrix.R.txt

Use of matrices

A Lotka-Volterra model with 4 species

```
> model <- function(t, n, parms) {
+   with(parms, {
+     dn <- r * n  + n * (A %*% n)
+     return(list(c(dn)))
+   })
+ }
> parms <- list(
+   r = c(r1 = 0.1, r2 = 0.1, r3 = -0.1, r4 = -0.1),
+   A = matrix(c(0.0, 0.0, -0.2, 0.0,      # prey 1
+                0.0, 0.0, 0.0, -0.1,      # prey 2
+                0.2, 0.0, 0.0, 0.0,       # predator 1; eats prey 1
+                0.0, 0.1, 0.0, 0.0),      # predator 2; eats prey 2
+                nrow = 4, ncol = 4, byrow = TRUE)
+ )

> system.time(out <- ode(n0, times, model, parms))

   user  system elapsed
   0.36    0.02    0.39
```

Source: examples/lv-plain-or-matrix.R.txt

Results

- `plot(out)` will show the results.
- Note that the "plain" version has only 1 to 1 connections, but the matrix model is already full connected (with most connections are zero). The comparison is insofar unfair that the matrix version (despite faster execution) is more powerful.
- Exercise: Create a fully connected model in the plain version for a fair comparison.
- A parameter example (e.g. for weak coupling) can be found on: http://tolstoy.newcastle.edu.au/R/e7/help/09/06/1230.html

Using compiled code

All solvers of deSolve

- allow direct communication between solvers and a compiled model.

See `vignette ("compiledCode")`

Principle

- Implement core model (and only this) in C or Fortran,
- Use data handling, storage and plotting facilities of R.

`examples/compiled_lorenz/compiledcode.svg`

[16] Soetaert, K., Petzoldt, T. and Setzer, R. (2009) R-package deSolve, Writing Code in Compiled Languages.

Thank you!

More Info:

`http://desolve.r-forge.r-project.org`

Citation

A lot of effort went in creating this software; please cite it when using it.

- deSolve: [22], rootSolve [21], ReacTran [18],
- Some complex examples can be found in [20],
- A framework to fit differential equation models to data is FME [19],
- ...and don't forget the authors of the original algorithms [5, 10, 2]!

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- Creation of the packages made use of R-Forge [23].

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