TECHNISCHE UNIVERSITÄT DRESDEN

A code generator for ODE-based models

–

R-package `rodeo`

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Special seminar of the Systems Analysis and Modelling group at EAWAG, 2016-05-03

Outline

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Background

- Lake eutrophication
- Flood management
- Operational runoff forecasting
- Early diagenesis of lake sediments
- Fate of antibiotic resistant bacteria

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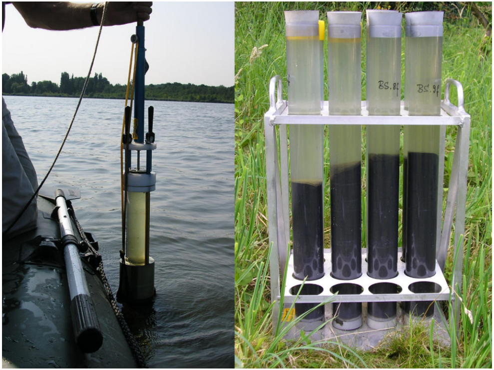

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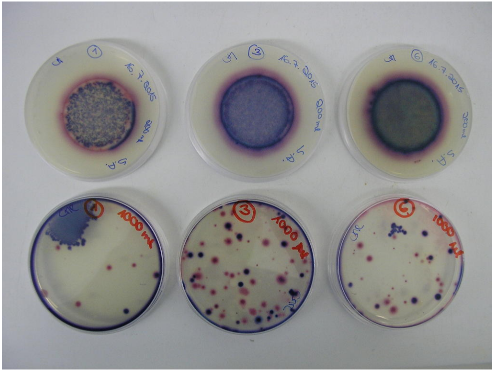

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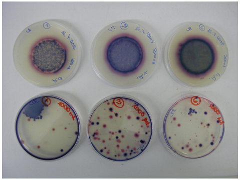


→ Several years of model/software development

Re-invention of the wheel?

- Best way to learn modeling is via model development.
- 'Monolithic codes' are hard to extend.
- Rising interest in structural uncertainty
  $\rightarrow$ Need for Re-implementations

Outline

Documentation

- Often incomplete or outdated
- Mistakes in published equations
- Source code alone not sufficient

$\rightarrow$ Embedded / automatic documentation

Portability & life time

- Implementation in specific language / framework
- Impedes collaborative development
- Software undergoes aging

$\rightarrow$ True portability

$\rightarrow$ Equations to be separated from source code

Handling of large arrays

- Access by index: Hard to read / maintain
- Access by name: Slow

$\rightarrow$ Combine the two options

Computational efficiency

- Interpreted code is convenient but relatively slow
- Need for high-performance (Optimization, Uncertainty, ...)

$\rightarrow$ Use compiled code sections

Redundant terms

- Repeated evaluation wastes time
- Code is difficult to maintain

$\rightarrow$ Use proper notation to reduce redundancies

$\rightarrow$ Let the compiler eliminate them

Various model interfaces

- Effort for users
- Individual pre-/post-processors
- Impedes coupling of models

$\rightarrow$ Unified interface

Wish list

- Built-in documentation
- True portability
- Save & fast array access
- Compiled code sections
- Less redundancies
- Unified interface

$\rightarrow$ `rodeo` is one attempt, among others, to achieve this

Scope

- Models built on simultaneous ODE

$$\frac{d}{dt}Y_1 = f(time, Y, parameters)$$

$$\dots$$

$$\frac{d}{dt}Y_n = f(time, Y, parameters)$$

- Numerical integration or steady-state estimation

Outline

Introduction

Objectives

Concepts

Minimalistic example

Specific features & limitations

Applications

Summary

Hands-on part

Two pillars

(1) Use of a table-based standard notation for ODE

- Built-in documentation
- Less redundancies
- Unified interface

Two pillars

(1) Use of a table-based standard notation for ODE

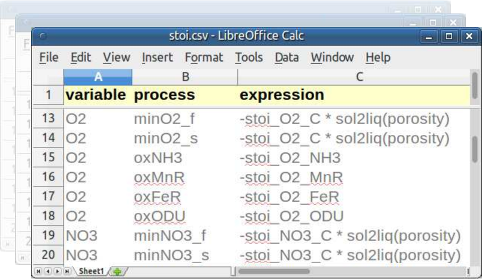
- Built-in documentation
- Less redundancies
- Unified interface

(2) Automatic code generation

- Save & fast array access
- Use of compiled code
- Portability

Overview

Table-based model definition



stoi.csv - LibreOffice Calc

	A	B	C
1	**variable**	**process**	**expression**
13	O2	minO2_f	-stoi_O2_C * sol2liq(porosity)
14	O2	minO2_s	-stoi_O2_C * sol2liq(porosity)
15	O2	oxNH3	-stoi_O2_NH3
16	O2	oxMnR	-stoi_O2_MnR
17	O2	oxFeR	-stoi_O2_FeR
18	O2	oxODU	-stoi_O2_ODU
19	NO3	minNO3_f	-stoi_NO3_C * sol2liq(porosity)
20	NO3	minNO3_s	-stoi_NO3_C * sol2liq(porosity)

→ *rodeo* object

Overview

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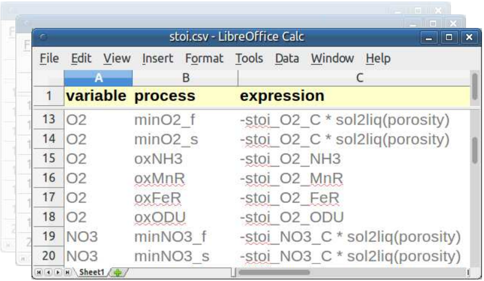

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15	O2	oxNH3	-stoi_O2_NH3
16	O2	oxMnR	-stoi_O2_MnR
17	O2	oxFeR	-stoi_O2_FeR
18	O2	oxODU	-stoi_O2_ODU
19	NO3	minNO3_f	-stoi_NO3_C * sol2liq(porosity)
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Components of *tex* or *html* documents

rodeo object

R code

Fortran code

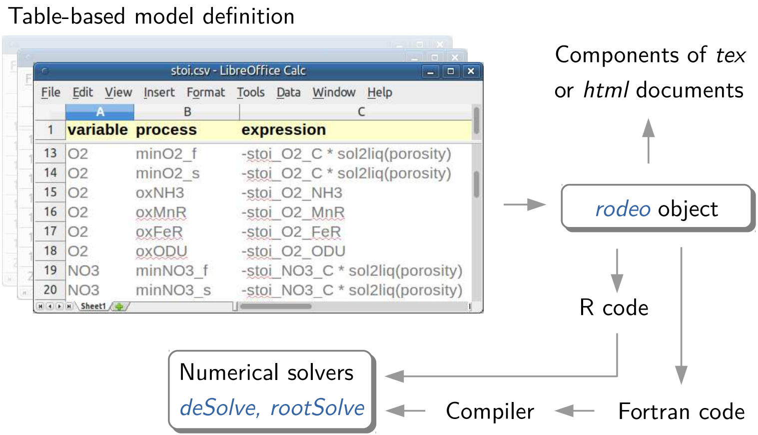
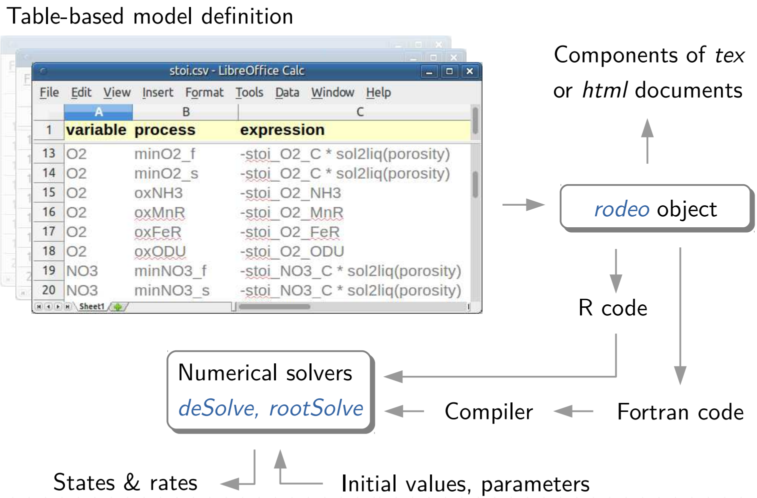


Table-based model definition
stoi.csv - LibreOffice Calc
File Edit View Insert Format Tools Data Window Help
variable process expression
13 O2 minO2_f -stoi_O2_C * sol2liq(porosity)
14 O2 minO2_s -stoi_O2_C * sol2liq(porosity)
15 O2 oxNH3 -stoi_O2_NH3
16 O2 oxMnR -stoi_O2_MnR
17 O2 oxFeR -stoi_O2_FeR
18 O2 oxODU -stoi_O2_ODU
19 NO3 minNO3_f -stoi_NO3_C * sol2liq(porosity)
20 NO3 minNO3_s -stoi_NO3_C * sol2liq(porosity)
Sheet1
Components of tex or html documents
rodeo object
R code
Numerical solvers
deSolve, rootSolve
Compiler
Fortran code

Overview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A B C
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16 O2 oxMnR -stoi_O2_MnR
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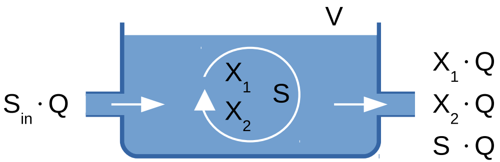
Fortran code
States & rates
Initial values, parameters

Outline

Modeled system

- Mixed reactor with constant volume V and flow rate Q
- Two species (X_1, X_2) competing for dissolved resource S



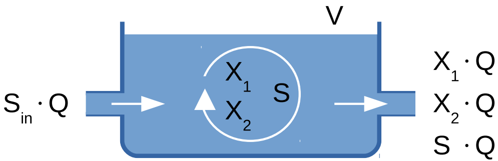
Corresponding ODE

$$\frac{d}{dt}X_1 = r_1 \cdot X_1 \cdot \frac{S}{S+h_1} - X_1 \cdot \frac{Q}{V}$$

$$\frac{d}{dt}X_2 = r_2 \cdot X_2 \cdot \frac{S}{S+h_2} - X_2 \cdot \frac{Q}{V}$$

$$\frac{d}{dt}S = -c_1 \cdot r_1 \cdot X_1 \cdot \frac{S}{S+h_1} - c_2 \cdot r_2 \cdot X_2 \cdot \frac{S}{S+h_2} + (S_{in} - S) \cdot \frac{Q}{V}$$

Growth
Im/Export



Matrix notation

$$\frac{d}{dt}X_1 = r_1 \cdot X_1 \cdot \frac{S}{S+h_1} - X_1 \cdot \frac{Q}{V}$$

$$\frac{d}{dt}X_2 = r_2 \cdot X_2 \cdot \frac{S}{S+h_2} - X_2 \cdot \frac{Q}{V}$$

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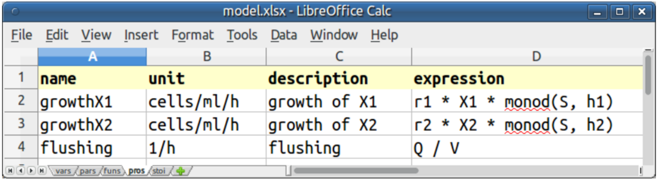
Growth

Im/Export

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ X_2 \\ S \end{bmatrix} = \begin{bmatrix} 1 & 0 & -X_1 \\ 0 & 1 & -X_2 \\ -c_1 & -c_2 & S_{in} - S \end{bmatrix} \cdot \begin{bmatrix} r_1 \cdot X_1 \cdot S/(S+h_1) \\ r_2 \cdot X_2 \cdot S/(S+h_2) \\ Q/V \end{bmatrix}$$

Table of Processes

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ X_2 \\ S \end{bmatrix} = \begin{bmatrix} 1 & 0 & -X_1 \\ 0 & 1 & -X_2 \\ -c_1 & -c_2 & S_{in} - S \end{bmatrix} \cdot \begin{bmatrix} r_1 \cdot X_1 \cdot S/(S + h_1) \\ r_2 \cdot X_2 \cdot S/(S + h_2) \\ Q/V \end{bmatrix}$$



model.xlsx - LibreOffice Calc

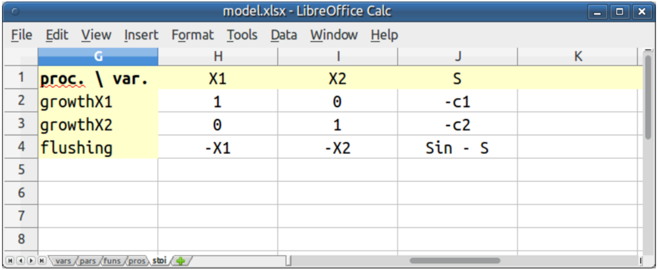
File Edit View Insert Format Tools Data Window Help

name	unit	description	expression
growthX1	cells/ml/h	growth of X1	r1 * X1 * monod(S, h1)
growthX2	cells/ml/h	growth of X2	r2 * X2 * monod(S, h2)
flushing	1/h	flushing	Q / V

vars pars funs pros stoi

Table of stoichiometric factors

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ X_2 \\ S \end{bmatrix} = \begin{bmatrix} 1 & 0 & -X_1 \\ 0 & 1 & -X_2 \\ -c_1 & -c_2 & S_{in} - S \end{bmatrix} \cdot \begin{bmatrix} r_1 \cdot X_1 \cdot S/(S + h_1) \\ r_2 \cdot X_2 \cdot S/(S + h_2) \\ Q/V \end{bmatrix}$$



	G	H	I	J	K
1	proc. \ var.	X1	X2	S	
2	growthX1	1	0	-c1	
3	growthX2	0	1	-c2	
4	flushing	-X1	-X2	Sin - S	
5					
6					
7					
8					

Tables with declarations

Variables

model.xlsx - LibreOffice Calc

name	unit	description	tex	html
X1	cells/ml	abundance species 1	X_1	X₁
X2	cells/ml	abundance species 2	X_2	X₂
S	mg/l	substrate	S	S

vars / pars / funs / pros / stoi

Parameters

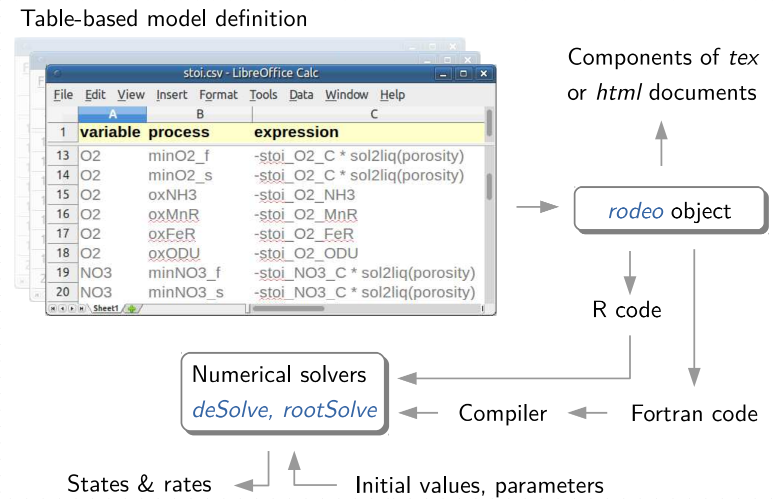
model.xlsx - LibreOffice Calc

name	unit	description	tex	html
r1	1/h	growth rate 1	r_1	r₁
r2	1/h	growth rate 2	r_2	r₂
h1	mg/ml	half sat. spec. 1	h_1	h₁
h2	mg/ml	half sat. spec. 2	h_2	h₂
c1	mg/cell	stoich. of X1	c_1	c₁
c2	mg/cell	stoich. of X2	c_2	c₂
Q	ml/h	flow rate	Q	Q
V	ml	volume	V	V
Sin	mg/ml	substrate in inflow	S_{in}	S_{in}

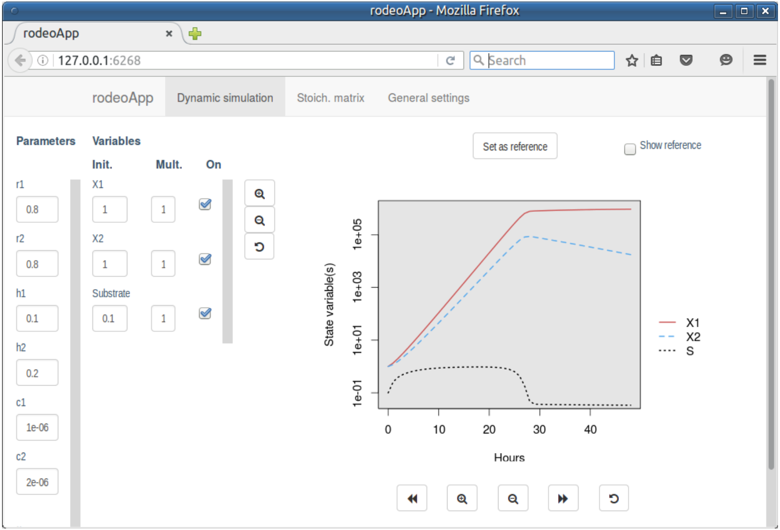
vars / pars / funs / pros / stoi

+ Functions

Code & document generation



Auto-generated GUI



Outline

Support for PDE

$$\frac{\partial c}{\partial t} = \underbrace{D \cdot \frac{\partial^2 c}{\partial x^2}}_{\text{Dispersion}} - \underbrace{u \cdot \frac{\partial c}{\partial x}}_{\text{Advection}} + \underbrace{R}_{\text{Reactions}}$$

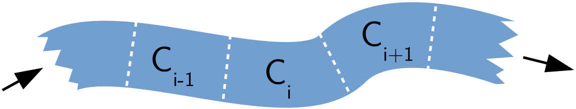
Support for PDE

$$\frac{\partial c}{\partial t} = \underbrace{D \cdot \frac{\partial^2 c}{\partial x^2}}_{\text{Dispersion}} - \underbrace{u \cdot \frac{\partial c}{\partial x}}_{\text{Advection}} + \underbrace{R}_{\text{Reactions}}$$

Method-of-lines

$$\frac{dc_i}{dt} = D \cdot \frac{(c_{i+1} - c_i) - (c_i - c_{i-1})}{\Delta x^2} - u \cdot \frac{c_i - c_{i-1}}{\Delta x} + R_i$$

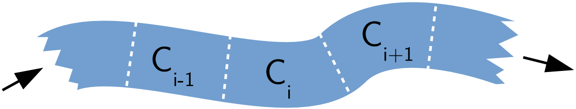
Support for PDE



Method-of-lines

$$\frac{dc_i}{dt} \quad = \quad D \cdot \frac{(c_{i+1} - c_i) - (c_i - c_{i-1})}{\Delta x^2} \quad - \quad u \cdot \frac{c_i - c_{i-1}}{\Delta x} \quad + \quad R_i$$

Support for PDE



Method-of-lines

$$\frac{dc_i}{dt} \quad = \quad D \cdot \frac{(c_{i+1} - c_i) - (c_i - c_{i-1})}{\Delta x^2} \quad - \quad u \cdot \frac{c_i - c_{i-1}}{\Delta x} \quad + \quad R_i$$

Function-like syntax to access adjacent cells, e.g.

```
u / dx * ( c - left(c) )
```

Forcing functions

`foo(time)` can appear in right hand side expressions

Actual functions must be defined

↙ ↘

Analytical

Interpolation

- Use `approxFun` in `R`-based models
- Use `rodeo`-generated Fortran code

Known limitations

- No forced documentation for user-function arguments
- No built-in support for 2D or 3D models
- Generated code uses a Fortran 2008 feature

Known limitations

CRAN Package Check Results for Package rodeo

Last updated on 2016-04-28 06:47:39.

Flavor	Version	$T_{install}$	T_{check}	T_{total}	Status	Flags
r-devel-linux-x86_64-debian-gcc	0.3	1.18	18.93	20.11	OK	
r-devel-linux-x86_64-fedora-clang	0.3			34.64	OK	
r-devel-linux-x86_64-fedora-gcc	0.3			22.28	OK	
r-devel-osx-x86_64-clang	0.3			37.30	OK	
r-devel-windows-ix86+x86_64	0.3	5.00	59.00	64.00	OK	
r-patched-linux-x86_64	0.3	1.19	18.58	19.77	OK	
r-patched-solaris-sparc	0.3			184.30	WARN	
r-patched-solaris-x86	0.3			41.20	WARN	
r-release-linux-x86_64	0.3	1.36	21.82	23.18	OK	
r-release-osx-x86_64-mavericks	0.3				OK	
r-release-windows-ix86+x86_64	0.3	5.00	72.00	77.00	OK	
r-oldrel-windows-ix86+x86_64	0.3	5.00	82.00	87.00	OK	

WARN: Compiler doesn't implement pointer initialization yet

Outline

`rodeo`-based projects

Existing

- Lake ecology (0D)
- Sediment diagenesis
- Dynamics of E. coli
- Prey-predator systems

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- Activated sludge model

`rodeo`-based projects

Existing

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Planned

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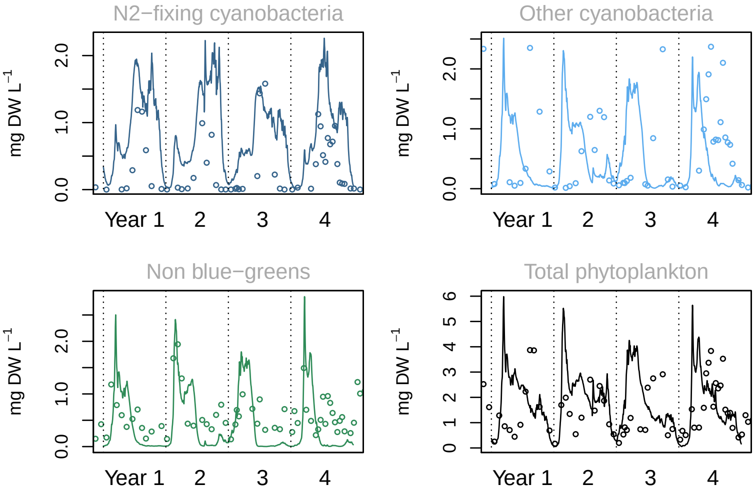
- Activated sludge model

Ecological lake model

- Heavily based on BELAMO
- Applied to a shallow lake, 1.3 km^2, z_{mean} 2.1 m

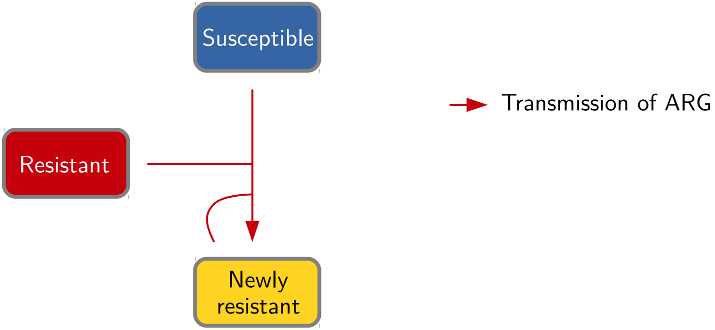
Contribution of N_2-fixation to Nitrogen balance?

Ecological lake model

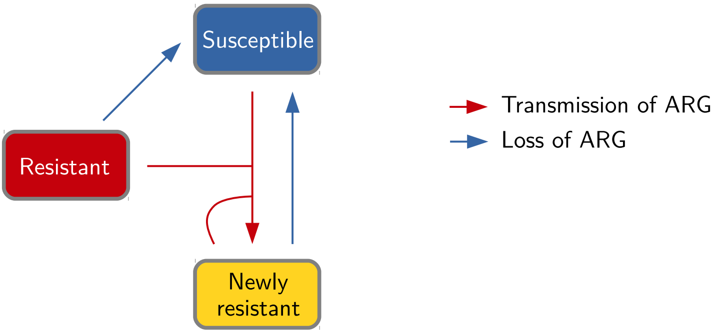


Data: BTU & WSA, Model: Omlin et al. (2001) modified by J. Feldbauer, M. Nisotaki, Y. Zhao

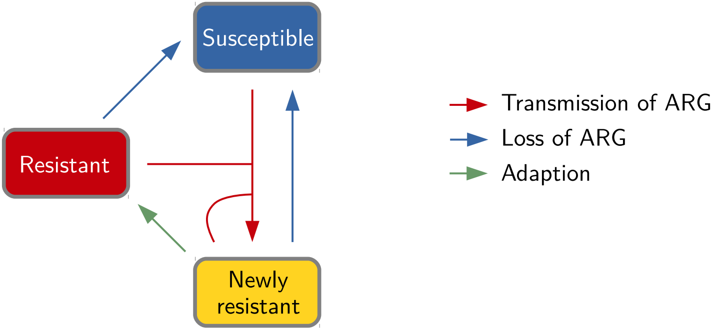
Antibiotic resistance



Antibiotic resistance



Antibiotic resistance



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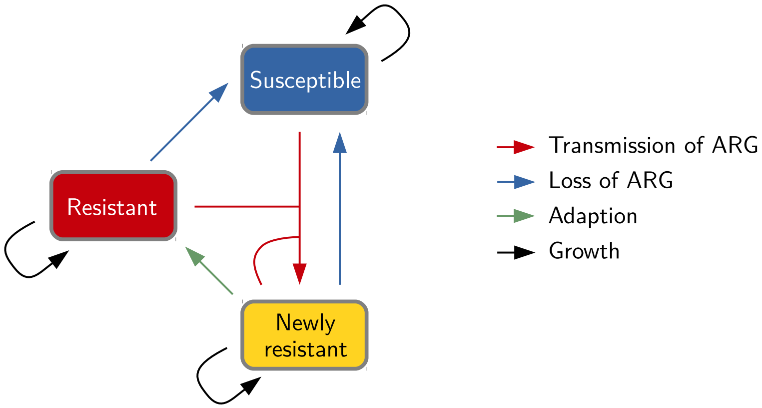

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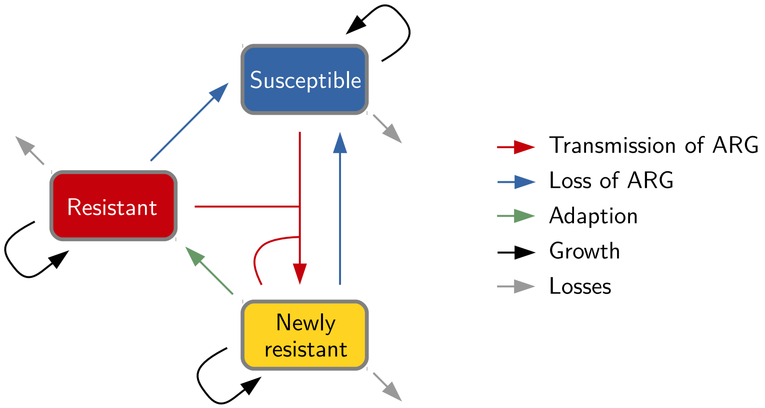

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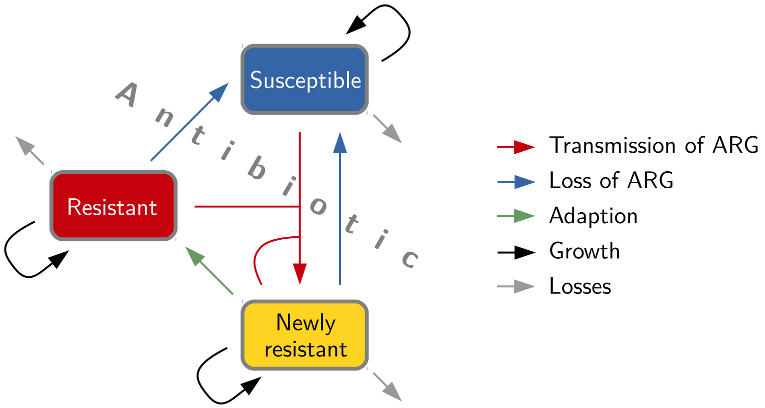
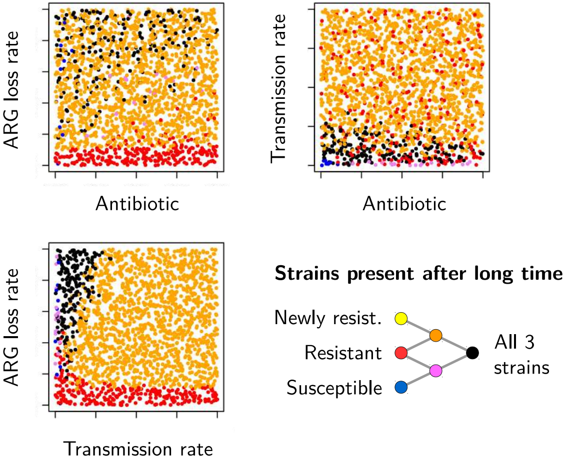
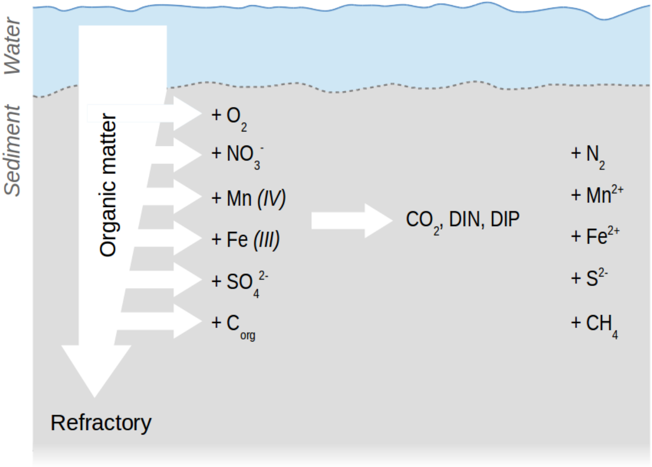


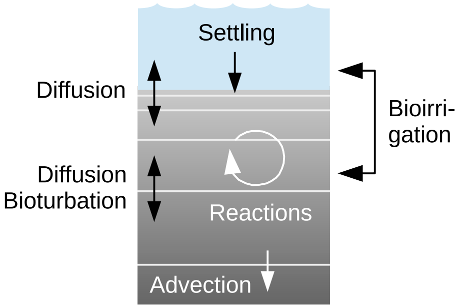
Antibiotic resistance



Early diagenesis



Early diagenesis



Early diagenesis

	C_{org}	DIP	IMP	NH_4^+	sorb. NH_4^+	NO_3^-	O_2	ODU
Settling	▲							
Mineral. (O_2)	▼	▲		▲			▼	
Mineral. (NO_3^-)	▼	▲		▲		▼		
Mineral. (anox.)	▼	▲		▲				▲
Nitrification				▼		▲	▼	
Oxidation w. O_2							▼	▼
Oxidation w. NO_3^-						▼		▼
P-Immobilization		▼	▲					
P-Remobilization		▲	▼					
NH_4^+-Sorption				▼	▲			
Advection ↓	●	●	●	●	●	●	●	●
Advection ↑		●		●		●	●	●
Diffus. transport	●	●	●	●	●	●	●	●
Diffus. at surface		●		●		●	●	●
Bioirrigation		●		●		●	●	●

Concentration

▲ increases

▼ decreases

● goes up or down

DIP: Dissolved inorg. P

IMP: Immobile inorg. P

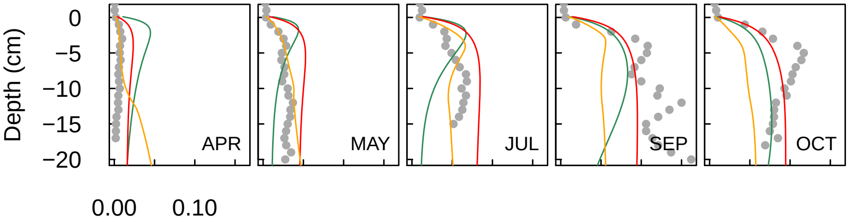
ODU: Mn^{2+}, Fe^{2+}, HS^-, ...

Basic concepts borrowed from Soetaert et al. (1996)

Early diagenesis

● Phosphorus in pore water, observed

/// Simulated with different model structures



mmol L^{-1}

Obs. data: Björn Grüneberg, BTU

Outline

Summary

Scope	Implementation of ODE models (+ 1D PDE)
Concepts	Table-based notation & code generation
Benefit	Simplicity and performance
Uses	Project work & teaching

Package	`https://cran.r-project.org/package=rodeo`
	`https://github.com/dkneis/rodeo`
Examples	`http://dkneis.github.io`
	`http://limno-live.hydro.tu-dresden.de/`

Thanks !

Sponsored by the Federal Ministry of Education and Research, Germany, Grant no. 0033W015EN, 02WU1351A

Outline

Required software

- Recent R version
- Developer tools (Rtools on Windows)
- R packages
  - `install.packages('deSolve')`
  - `install.packages('readxl')`
  - `install.packages('rodeo')`

Link to instructions on http://dkneis.github.io

`rodeo` objects

https://cran.r-project.org/package=rodeo

- `rodeo` class is a 'reference class'
- Creation: `object <- new('rodeo', <data>)`
- Usage: `object$method()`

`rodeo` objects

https://cran.r-project.org/package=rodeo

- `rodeo` class is a 'reference class'
- Creation: `object <- new('rodeo', <data>)`
- Usage: `object$method()`

```
install.packages('rodeo')   # done this already?
library('rodeo')
?rodeo
vignette('rodeo')
```

`deSolve` integrators

https://cran.r-project.org/package=deSolve

- Switch between stiff and non-stiff methods
- Structure of Jacobian can be specified
- Works with compiled code in shared library

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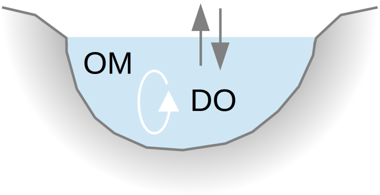
```
install.packages('deSolve')   # done this already?
library('deSolve')
?lsoda
?ode
```

Demo examples

- See links on http://dkneis.github.io
- Available in latest `rodeo` package (not on CRAN yet)

Streeter-Phelps

OM	Organic matter (mg/L)
DO	Dissolved oxygen (mg/L)



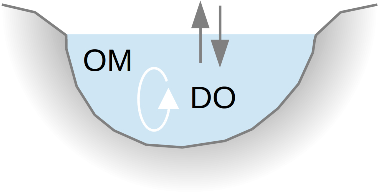
Streeter, W. H. and Phelps, W. B. (1925): A study of the pollution and natural purification of the Ohio River. Public Health Bull. 146, US Public Health Service, Washington DC.

→ Essential extensions developed in past 90 years

Streeter-Phelps

$$\frac{d}{dt}OM = -\, k_d \cdot OM$$

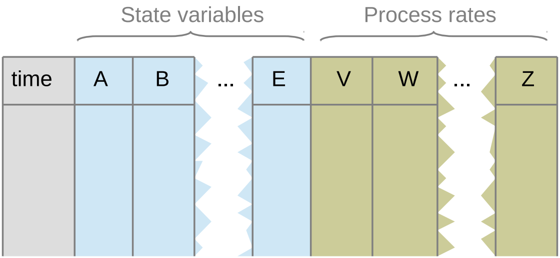
$$\frac{d}{dt}DO = -\, k_d \cdot OM \cdot s + k_a \cdot (DO_{sat} - DO)$$



Symbol	Units	Descr.
k_d	d^{-1}	Decay rate
k_a	d^{-1}	Aeration rate
s	Mass ratio	DO consumed per degraded OM
DO_{sat}	mg/L	O_2 saturation level

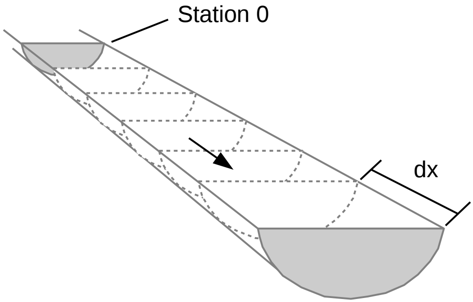
Streeter-Phelps

`deSolve` output for 0D `rodeo` models

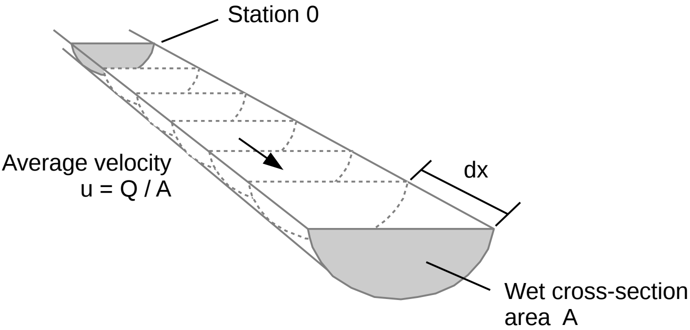



```
is.matrix(out)   # TRUE
ncol(out) == 1 + m$lenVars() + m$lenPros()   # m: model
colnames(out) == c('time', m$namesVars(), m$namesPros())
```

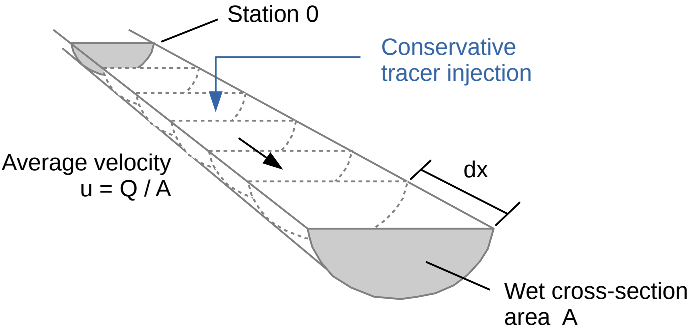
Advection-dispersion



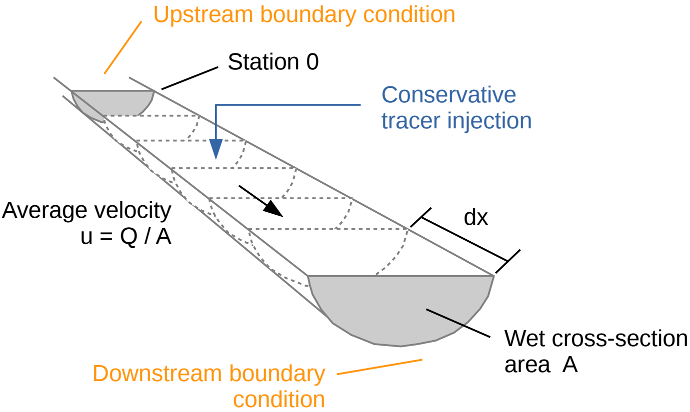
Advection-dispersion



Advection-dispersion

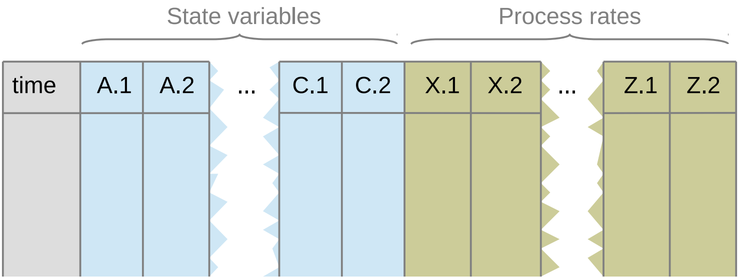


Advection-dispersion



Advection-dispersion

`deSolve` output for 1D `rodeo` models




```
ncol(out) == 1 + m$lenVars() * nBox + m$lenPros() * nBox
```

Advection-dispersion

`deSolve` output for 1D `rodeo` models

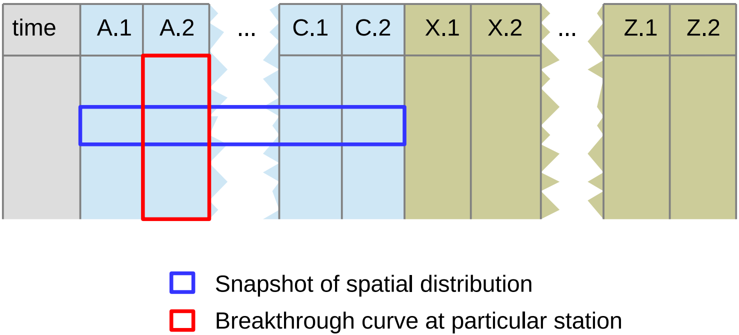


Table file formats

Delimited text	▸ Powerful editors (regular exp., syntax highlight) ▸ Version control ▸ Many processing options (LaTeX, data base, ...) ▸ Portable (but newline & encoding issues)
Spreadsheet	▸ Tabular view ▸ All tables kept in a single file ▸ Portable (different issues)

$\rightarrow$ Best used in combination