Phytoplankton, Microcosms, ODE's, R.

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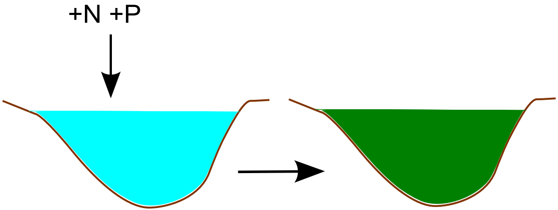
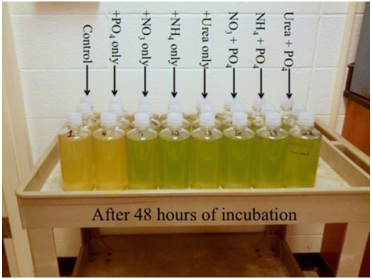
useR-Aalborg 01 July 2015

Ecology

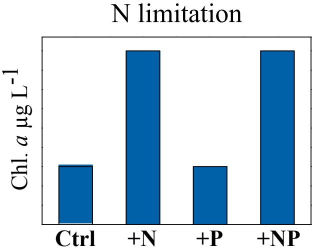
Eutrophication



Bioassays

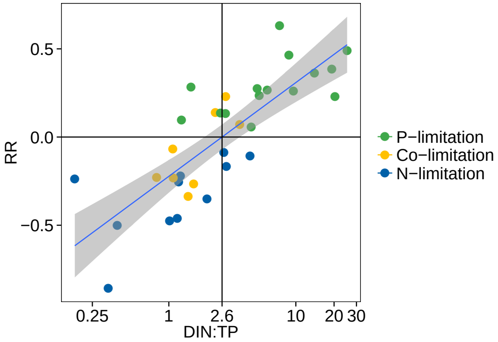


Davis et al (2015)



Kolzau et al (2014)

Standard statistics



Kolzau et al (2014)

$$RR = log(P_{response}/N_{response})$$

ODE's

Simulate the microcosm with ODE's

Phytoplankton (C_{phy}) + 1 resource (N_{phy} and DIN)

$$\frac{dC_{phy}}{dt} = \frac{C_{phy}\, IN_{max} \left(1 - \frac{C_{phy}\, IN_{min}}{N_{phy}}\right)}{IN_{max} - IN_{min}}$$

$$\frac{dN_{phy}}{dt} = \frac{C_{phy} \left(IN_{max} - \frac{N_{phy}}{C_{phy}}\right) Nup_{max}\, DIN}{(IN_{max} - IN_{min}) \left(DIN + K_{Nup}\right)}$$

$$\frac{dDIN}{dt} = -\left\{\frac{C_{phy} \left(IN_{max} - \frac{N_{phy}}{C_{phy}}\right) Nup_{max}\, DIN}{(IN_{max} - IN_{min}) \left(DIN + K_{Nup}\right)}\right\}$$

Use numerical solvers to step forward in time from initial conditions.

Technical challenges

- No standard implementation
  - Sharing (communication between modellers) is difficult
  - Re-use is difficult
  - No standard = hard to get started
- Theory and code entangled
  - Poor documentation
  - Collaboration with non-modellers is difficult

rodeo

Definition in tables + Code generation

rodeo - David Kneis

https://github.com/dkneis/rodeo

Identifiers

	name	type	unit	description	tex	html
1	C_phy	v	µgC/L	Cellular C	C_{phy}	C_phy
2	N_phy	v	µgN/L	Cellular N	N_{phy}	N_phy
3	DIN	v	µgN/L	External dissolved inorganic N	DIN	DIN
4	r_max	p	1/day	Max phytoplankton growth rate	r_{max}	r_max
5	IN_max	p	gN/gC	Max internal N:C ratio	IN_{max}	IN_max
6	IN_min	p	gN/gC	Min internal N:C ratio	IN_{min}	IN_min
7	UN_max	p	gN/gC/day	Max N uptake rate	UP_{max}	UN_max
8	K_Nup	p	µgN/L	Half sat. for N uptake	K_{Nup}	K_Nup
9	uptake	f	µg/µgC/d	uptake rate for N	uptake	uptake
10	droop	f	µgC/µgC/d	realised growth rate of phytoplankton	droop	droop

Processes

	name	unit	description	expression
1	Growth	µgC/d	Growth	r_max * droop(IN_max, IN_min, N_phy/C_phy)
2	U_DIN	µgN/d	Uptake of DIN	uptake(UN_max, IN_max, IN_min, K_Nup, DIN, N_phy/C_phy)

Stoichiometry

	variable	process	expression
1	C_phy	Growth	C_phy
2	N_phy	U_DIN	C_phy
3	DIN	U_DIN	−C_phy

Define functions

```
uptake <- function(Umax, Qmax, Qmin, K_half, Ext, Int)
  {Umax*((Ext*(Qmax-Int))/((K_half+Ext)*(Qmax-Qmin)))}

droop <- function(Qmax, Qmin, Int)
  {(Qmax / (Qmax - Qmin)) * (1 - (Qmin / Int))}
```

Neat documentation

State variables

Symbol	Unit	Description
C_{phy}	µgC/L	Cellular C
N_{phy}	µgN/L	Cellular N
DIN	µgN/L	External dissolved inorganic N

Parameters

Symbol	Unit	Description
r_{max}	1/day	Max phytoplankton growth rate
IN_{max}	gN/gC	Max internal N:C ratio
IN_{min}	gN/gC	Min internal N:C ratio
UP_{max}	gN/gC/day	Max N uptake rate
K_{Nup}	µgN/L	Half sat. for N uptake

Code generation

Instantiate model object

```
model <- new("rodeo", vars=subset(identifiers,type=="v")
             , pars=subset(identifiers,type=="p")
             , funs=subset(identifiers,type=="f")
             , pros=processes, stoi=stoichiometry)
```

Generate code

R or Fortran95

```
code <- model$generate(name="derivs",lang="r")
derivs <- eval(parse(text=code))
```

Provide parameter and starting values

```
pars <- list(r_max=1, K_Nup=100, UN_max=0.2
             , IN_max=0.13 * (14/12)
             , IN_min=0.05 * (14/12))

init_C_phy <- 2000
init_DIN <- 80

vars <- list(C_phy=init_C_phy, DIN=init_DIN
             , N_phy=(2*pars[["IN_min"]])*init_C_phy)

p <- model$arrangePars(pars)
v <- model$arrangeVars(vars)
```

Test the derivative function

```
derivs(time, v, p, NLVL = 1)
```

```
## $dydt
## [1] 1625.00000   66.66667  -66.66667
##
## $pro
## [1] 0.81250000 0.03333333
```

deSolve

Solve the ODE system

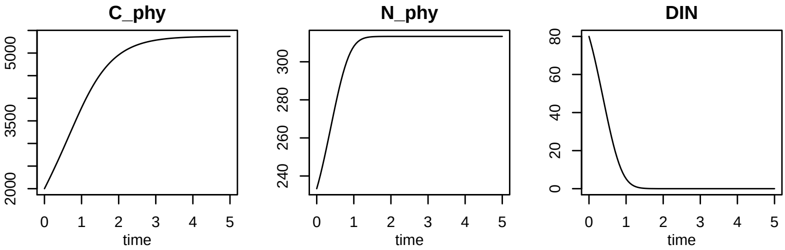
Pass parameters and starting values at runtime

```
t <- seq(0, 5, length.out=100)

system.time({
  out_R1 <- ode(y=v, times=t, func=derivs
                , parms=p, NLVL=1)
})
```

```
##     user  system elapsed
##     0.06    0.00    0.08
```

Plot output


C_phy
5000
3500
2000
0
1
2
3
4
5
time
N_phy
300
280
260
240
0
1
2
3
4
5
time
DIN
80
60
40
20
0
0
1
2
3
4
5
time

Shiny!

More ecology

- N **or** P limit growth rate
- Effect of light (I) is multiplicative

$$\frac{dC_{phy}}{dt} = f(I) \cdot min\{f(N), f(P)\}$$

Shiny app demonstration

Packages

- rodeo (David Kneis) `https://github.com/dkneis/rodeo`
  - Standard definition of ODE's in tables
  - Definition is the documentation
  - Code generation in R or F95 (250x faster)
- deSolve (Soetaert, Petzoldt, Setzer)
  - Numeric solvers for DE
- Shiny (Chang, Cheng, Allaire, Xie and McPherson)

Acknowledgments

- David Kneis *rodeo* @TU Dresden
  - `https://github.com/dkneis/rodeo`
- Thomas Petzoldt @TU Dresden
- Sebastian Kolzau, Jacqueline Rücker, Claudia Wiedner @BTU
- Nitrolimit www.nitrolimit.de
- BMBF FONA 033L041A and 0033W015AN

NITROLIMIT

b-tu Brandenburg University of Technology Cottbus - Senftenberg

Petersen matrix

$$
\begin{array}{l}
\text{Growth} \\
\text{U DIN}
\end{array}
\overset{\begin{array}{ccc} C_{phy} & N_{phy} & DIN \end{array}}{\begin{pmatrix} C_{phy} & 0 & 0 \\ 0 & C_{phy} & -C_{phy} \end{pmatrix}}
\quad
\overset{\text{Rate expressions}}{\begin{pmatrix} f(\frac{N_{phy}}{C_{phy}}, IN_{max}, IN_{min}) \\ f(DIN, \frac{N_{phy}}{C_{phy}}, Nup_{max}, \ldots) \end{pmatrix}}
$$

Literature cited

- Davis, T.W., Bullerjahn, G.S., Tuttle, T., McKay, R.M. & Watson, S.B. (2015) Effects of Increasing Nitrogen and Phosphorus Concentrations on Phytoplankton Community Growth and Toxicity During Planktothrix Blooms in Sandusky Bay, Lake Erie. Environmental Science & Technology, 49, 7197–7207.
- Karline Soetaert, Thomas Petzoldt, R. Woodrow Setzer (2010). Solving Differential Equations in R: Package **deSolve** Journal of Statistical Software, 33(9), 1–25. URL `http://www.jstatsoft.org/v33/i09/`.

- Kolzau, S., Wiedner, C., Rücker, J., Köhler, J., Köhler, A. & Dolman, A.M. (2014) Seasonal patterns of nitrogen and phosphorus limitation in four German lakes and the predictability of limitation status from ambient nutrient concentrations. PLoS ONE, 9, e96065.