Exercise 1

Modelling Aquatic Ecosystems FS24

Who are we?

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We are in charge of:

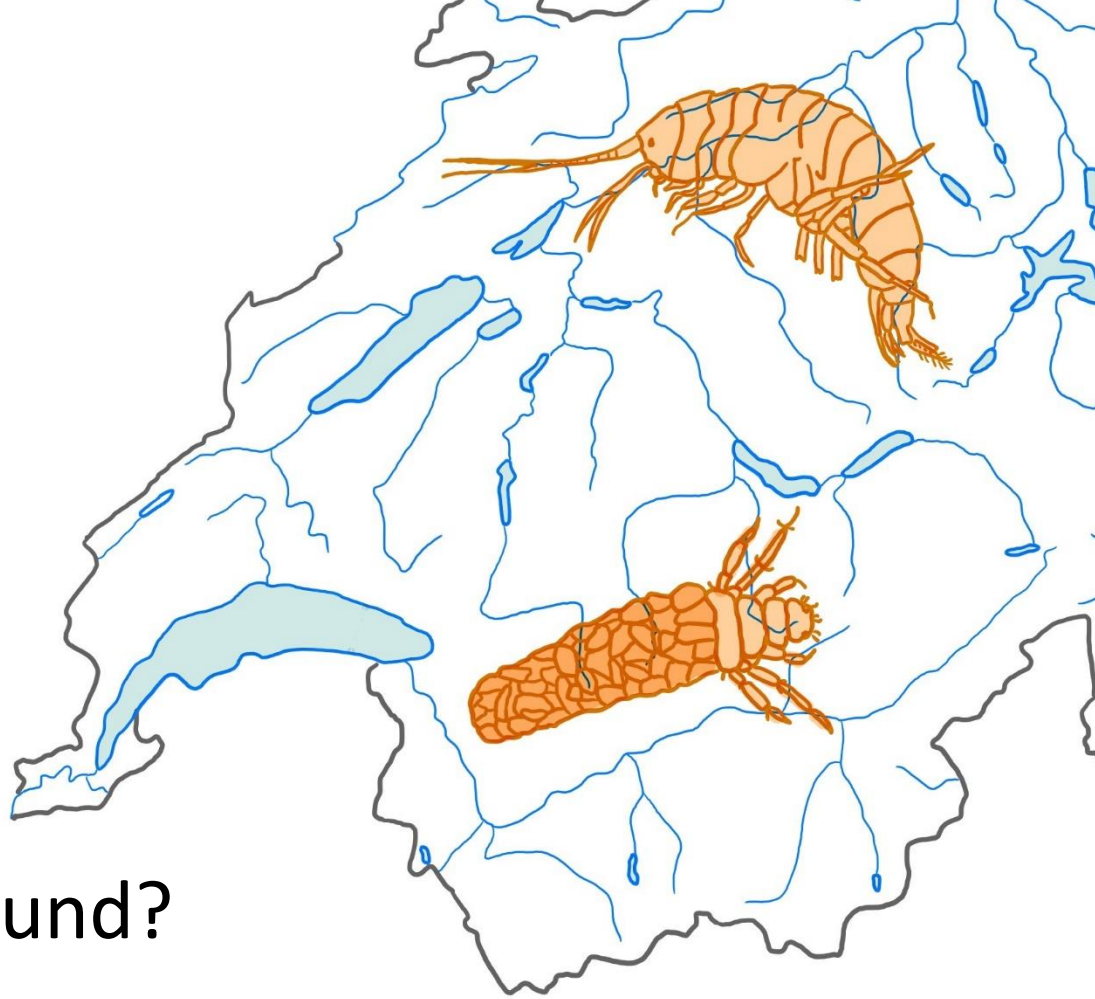
- Exercises
- Modelling project

Don’t hesitate to ask questions and give feedback!

We speak English, Mandarin and French

Who are you?

- What is your study background?
- What is your programming background?



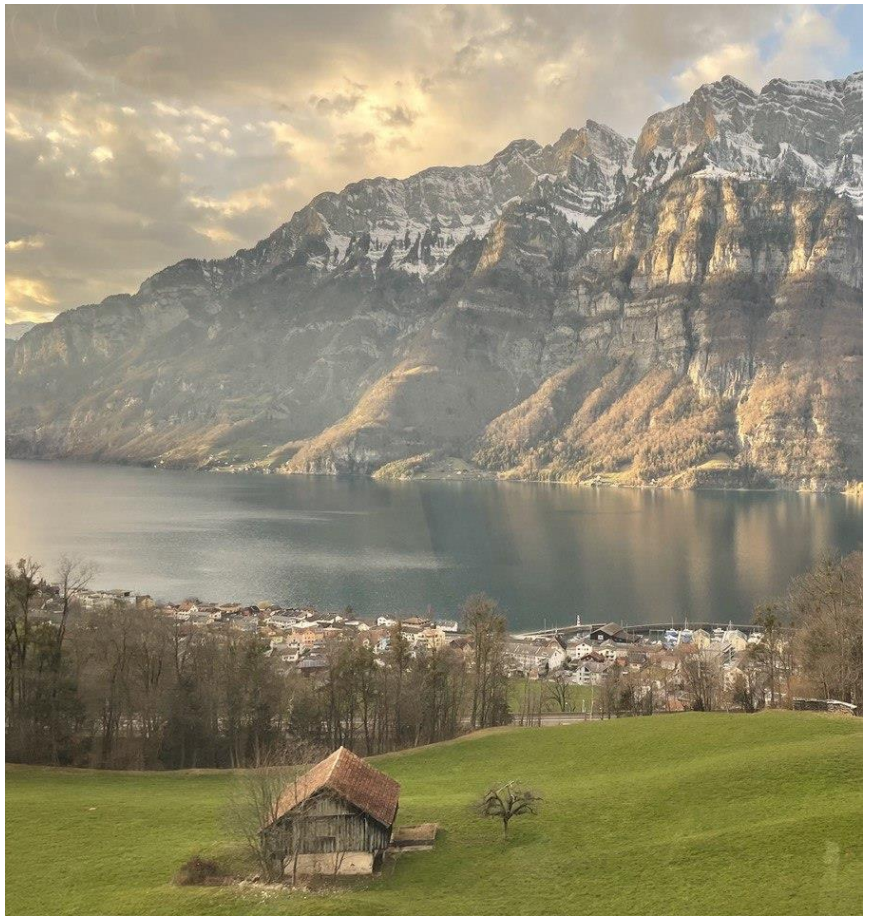
Goals of the exercises

- Deepen and extend the knowledge gained in the lectures through simulation and sensitivity analysis of aquatic ecosystem models.

- Learn to implement and use models with R and extensions in the form of packages.

Today's agenda

- Recap of theory
- Intro to R and R Markdown
- Work on the exercise
- Break
- Intro to R package ecosim
- Work on the exercise
- Discussion of theory questions



Walensee, St-Gallen

Define the physical environment, its variables and processes

Mixed reactor of constant volume - Epilimnion

Inputs

Q_{in}: Inflow

$C_{\mathrm{HPO4,in}}$: Phosphate

In-box variables

V: Volume

C_{HPO4}: Phosphate

C_{ALG}: Algae

$r_{\mathrm{HPO4}}, r_{\mathrm{ALG}}$: Total transformation rates

Ecological processes

Growth algae

Death algae

Output

Q_{out}: Outflow (with phosphate and algae)

Write down the differential equations

Time dependent state variables ~ Corresponds to the substances/organisms you want to model

$$\frac{\mathrm{d}C_{\mathrm{HPO4}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right) + r_{\mathrm{HPO4}}$$

$$\frac{\mathrm{d}C_{\mathrm{ALG}}}{\mathrm{d}t} = -\frac{Q_{\mathrm{in}}}{V}C_{\mathrm{ALG}} + r_{\mathrm{ALG}}$$

Transformation rates ~ Includes ecological processes of the model

Recap – Process table, process rates and limitation factors

Write down the process table

- the ecological processes
- the substances/organisms
- the stoichiometric coefficients
- the process rates

Process	Substances / Organisms HPO4 [gP/m³]	ALG [gDM/m³]	Rate
Growth of algae	$-\alpha_{\mathrm{P,ALG}}$	1	$\rho_{\mathrm{gro,ALG}}$
Death of algae		-1	$\rho_{\mathrm{death,ALG}}$

Write down the process rates

- specific growth rate
- limitation by substance concentrations
- inhibition by substance concentrations
- temperature/light dependence
- substance concentration

Rate	Rate expression
$\rho_{\mathrm{gro,ALG}}$	$k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}} C_{\mathrm{ALG}}$
$\rho_{\mathrm{death,ALG}}$	$k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$

Calculate the total transformation rates

- multiply the stoichiometric coefficients with the process rates
- for each substance sum the contribution of all processes

Process Table × Rates	Total transformation rate
$1 \times \rho_{\mathrm{gro,ALG}} - 1 \times \rho_{\mathrm{death,ALG}}$	$= r_{C_{\mathrm{ALG}}}$
$-\alpha_{\mathrm{P,ALG}} \times \rho_{\mathrm{gro,ALG}}$	$= r_{C_{\mathrm{HPO4}}}$

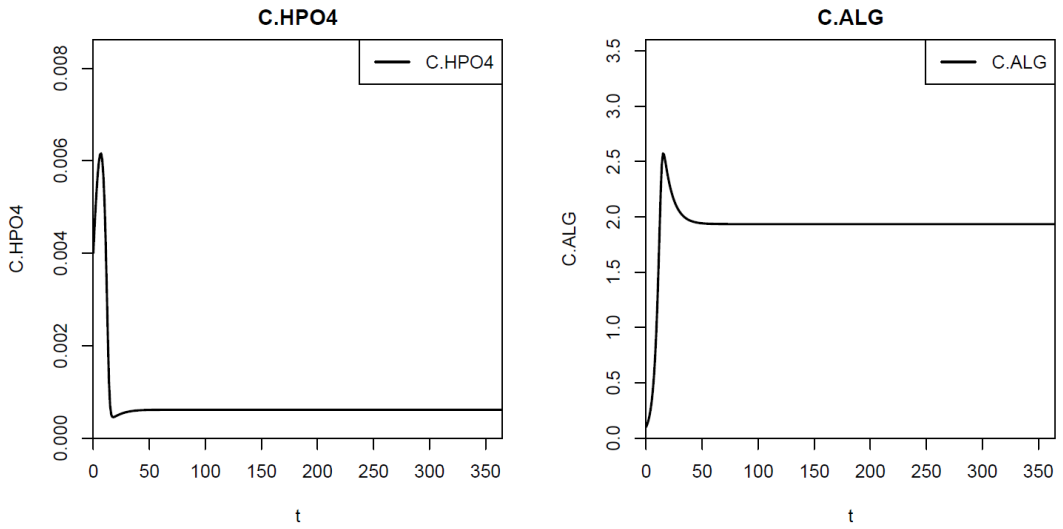
Replace them in the differential equations

$$\frac{\mathrm{d}C_{\mathrm{HPO_4^{2-}}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{in,HPO_4^{2-}}} - C_{\mathrm{HPO_4^{2-}}}\right) - \alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}} C_{\mathrm{ALG}}$$

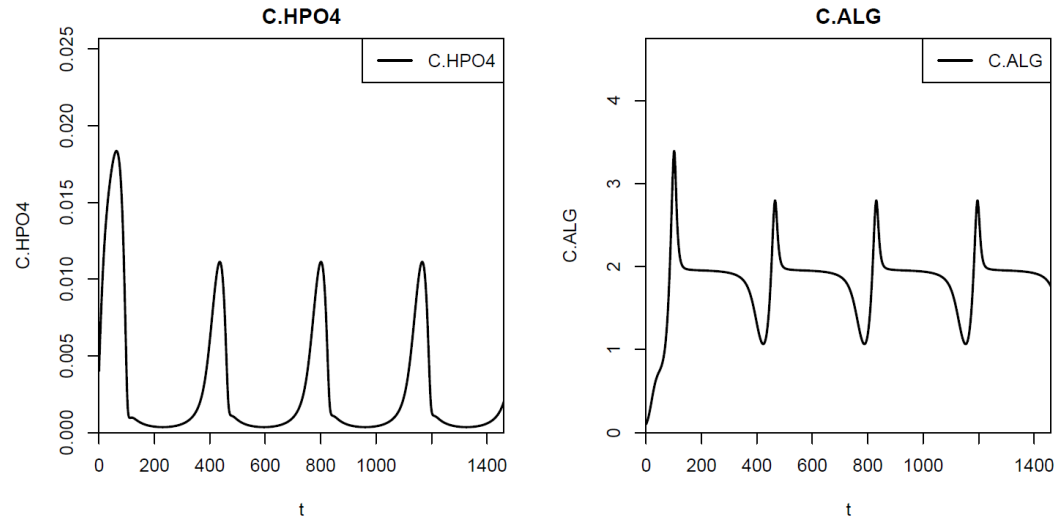
$$\frac{\mathrm{d}C_{\mathrm{ALG}}}{\mathrm{d}t} = -\frac{Q_{\mathrm{in}}}{V} C_{\mathrm{ALG}} + k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}} C_{\mathrm{ALG}} - k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$$

Code all these steps (in R), run simulations, visualize and analyze results!

One year simulation of HPO4 and ALG concentrations with **constant** driving forces

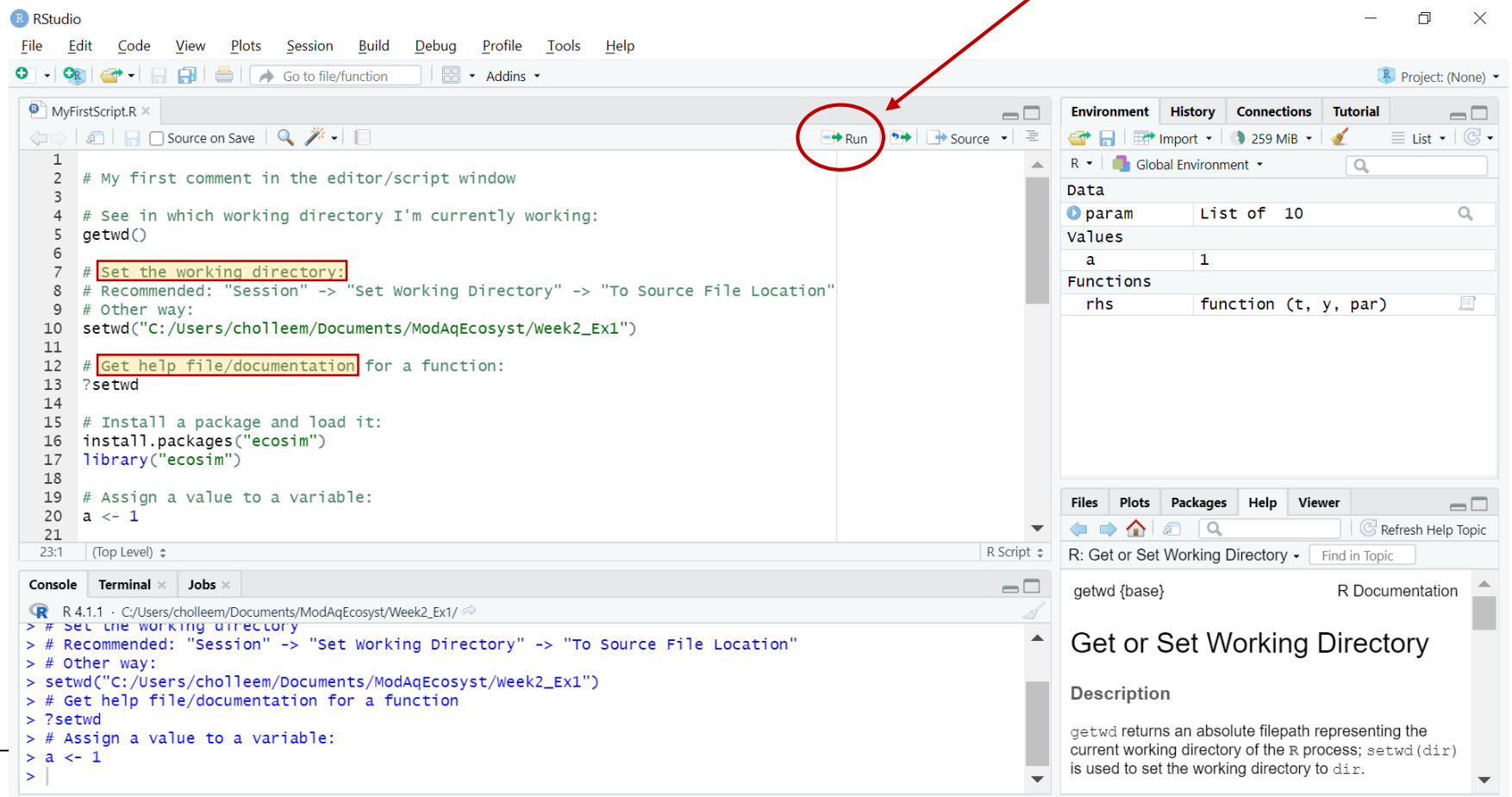


Four years simulation of HPO4 and ALG concentrations with **periodic** driving forces (temperature and light)



Intro to R

Editor/scripts (.R):
- Collection of commands
- Can be edited and saved
- Lines executed by pressing “Run” or “CTRL + ENTER”



Environment:
- See data and values in R memory

Viewer:
- Open files
- View plots
- Install and load packages
- Use/see help functions

Console:
- Type commands
- Executed by pressing “ENTER”
- Where R actually does stuff

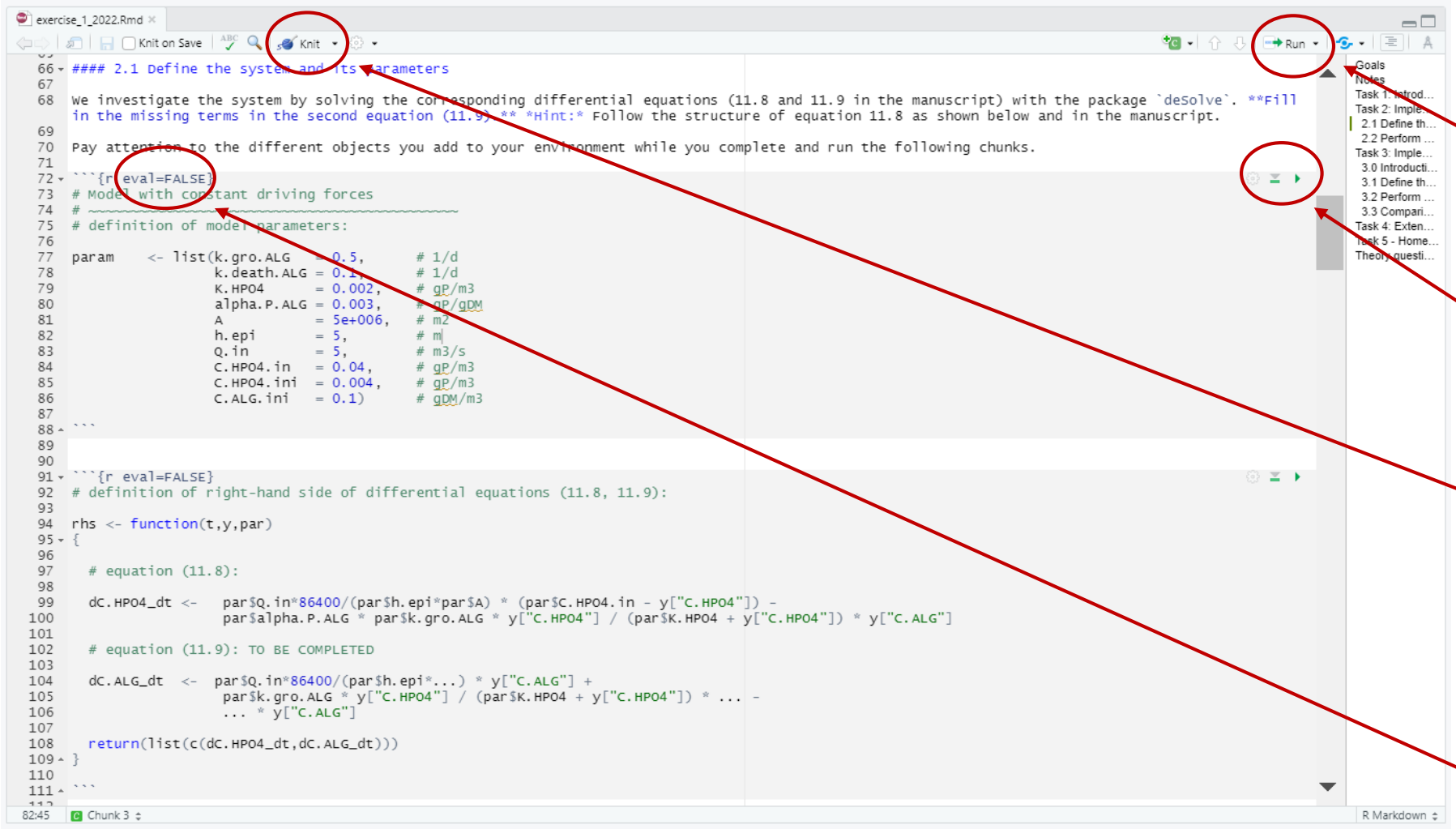
Intro to R Markdown

R Markdown file (.Rmd):

- Written in markdown
- Contains chunks of R code embedded by typing:

```
```{r}

```
```



Run current chunk:

- Press “Run” -> “Run current chunk”
- Or “CTRL + SHIFT + ENTER”
- Or green arrow

Produce a document:

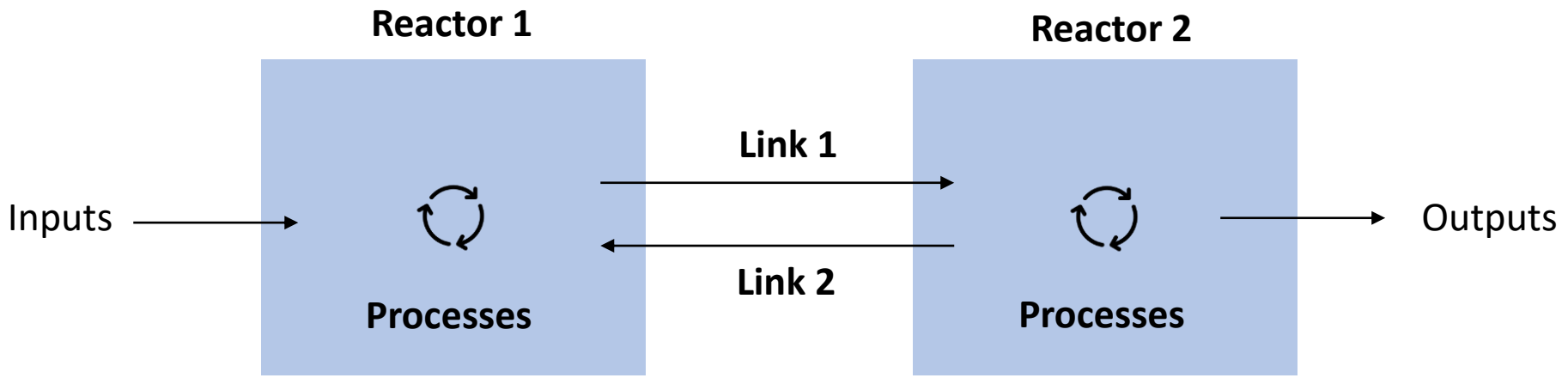
- Press “Knit” to produce an HTML, PDF or Word file
- It will be saved in your current Working Directory
- Set “eval” to TRUE to run the chunks

Work on **Task 2** of Exercise 1

Ecosim package

- Define a model using **classes:**
  - Arbitrary inputs and transformation **processes,**
  - Embedded in well-mixed **reactors,**
  - Connected by **links** (diffusive, advective),
  - All defined in a **system.**

Perform dynamic simulations, whose results can be plotted.



Ecosim package - Processes are defined by…

- A name
- A process rate
- A substance specific stoichiometric coefficient

```
# definition of transformation processes

# growth of algae:

gro.ALG   <- new(Class  = "process",
                 name   = "Growth of algae",
                 rate   = expression(k.gro.ALG
                                     *C.HPO4/(K.HPO4+C.HPO4)
                                     *C.ALG),
                 stoich = list(C.ALG  = expression(1),                # gDM/gDM
                               C.HPO4 = expression(-alpha.P.ALG)))  # gP/gDM
```

Ecosim package - Reactors consist of…

- A name
- Dimensions (height, area –> volume)
- Initial and inflow concentrations
- Inflows and outflows
- Processes

```
# definition of reactor to describe the epilimnion of the lake:

epilimnion <-
   new(Class             = "reactor",
       name              = "Epilimnion",
       volume.ini        = expression(A*h.epi),
       conc.pervol.ini   = list(C.HPO4 = expression(C.HPO4.ini),
                                C.ALG  = expression(C.ALG.ini)),
       inflow            = expression(Q.in*86400),
       inflow.conc       = list(C.HPO4 = expression(C.HPO4.in),
                                C.ALG  = 0),
       outflow           = expression(Q.in*86400),
       processes         = list(gro.ALG,death.ALG))
```

Ecosim package - Systems consist of…

- A name
- The reactors
- (Links, if there are multiple reactors)
- The parameters
- T.out

```
# definition of the system consisting of a single reactor:

system.11.1.a <- new(Class    = "system",
                     name     = "Lake",
                     reactors = list(epilimnion),
                     param    = param,
                     t.out    = seq(0,365,by=1))
```

Ecosim package – Important functions

- calcres → performs simulation of the model described by a system
- plotres → plots and helps to vizualize all the results
- calcsens → performs sensitivity analyses (that can then be plotted with plotres)

A **sensitivity analysis** is an analysis of how sensitive the model results are to changes in the parameter values.

The simplest way of doing this is a so called **"local sensitivity analysis"**, where **we change just one parameter at a time** and keep the **other parameters fixed**, run the model and plot and analyze the results.

More information on Ecosim in Chapter 16 of the manuscript.

Remark on object-oriented programming

Note the system contains all definitions of reactors, processes, model parameters and the output time points.

Any simulation carried out will refer to the definitions in the system, and not to the external variables that were used to set up the elements of the system.

Thus, if you **change a value** in a process, reactor or a parameter, you need to **re-create or update the system object** .

Work on **Task 3 and 4** of Exercise 1

Question 1

How can you derive the total (net) transformation rate of $C_{\mathrm{HPO_4^{-2}}}$ and C_{ALG} from the process table (Table 11.1) and the process rates (Table 11.2)?

Hint: see equation (4.1) in the manuscript. What are the units?

Question 1

Process Table

Process	Substances / Organisms HPO4 [gP/m^3]	ALG [gDM/m^3]	Rate	
Growth of algae	$-\alpha_{\mathrm{P,ALG}}$	1	$\rho_{\mathrm{gro,ALG}}$	= $k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}} C_{\mathrm{ALG}}$
Death of algae		-1	$\rho_{\mathrm{death,ALG}}$	= $k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$

$$r_j = \sum_{i=1}^{n_{\mathrm{P}}} \nu_{ij} \rho_i$$

r = Net transformation rate

ν = Substance-specific stoichiometric coefficients

ρ = Process rate

j = Substance

i = Process

Question 1

Solution:

$$r_{Alg} = k_{gro,\,Alg} \times \frac{C_P}{K + C_P} \times C_{Alg} - k_{death,\,Alg} \times C_{Alg}$$

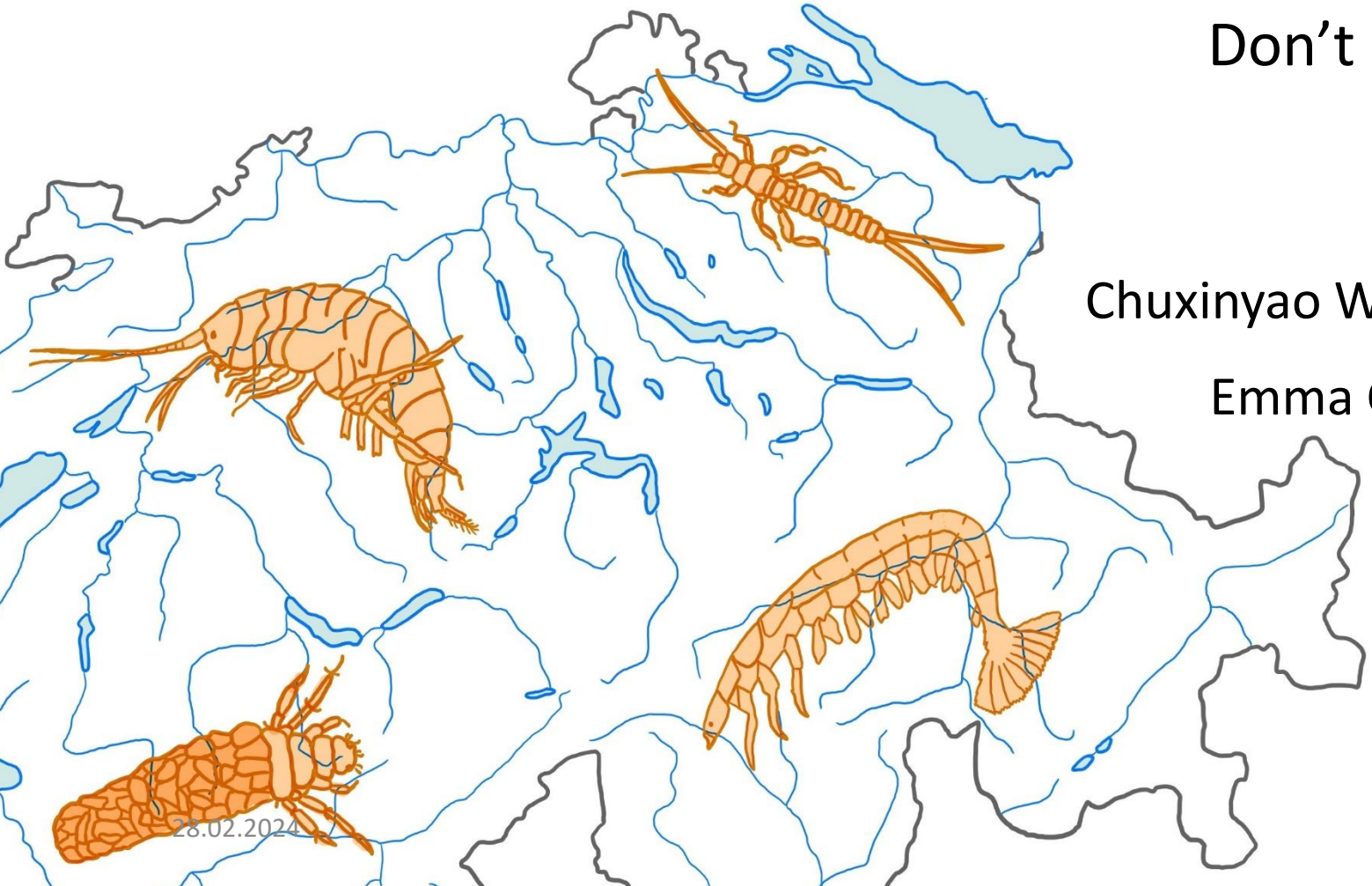
$$[r_{Alg}] = \frac{1}{d} \times \frac{gDM}{m^3} = \frac{gDM}{d \times m^3}$$

$$r_P = -\alpha_{P,Alg} \times k_{gro,\,Alg} \times \frac{C_P}{K + C_P} \times C_{Alg}$$

$$[r_P] = \frac{gP}{gDM} \times \frac{1}{d} \times \frac{gDM}{m^3} = \frac{gP}{d \times m^3}$$

Homeworks:

- Task 5 – Sensitivity analysis
- Question 2



Don’t hesitate to send us an e-mail if you have any questions.

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Have a nice sunny day !