

# Exercise 3

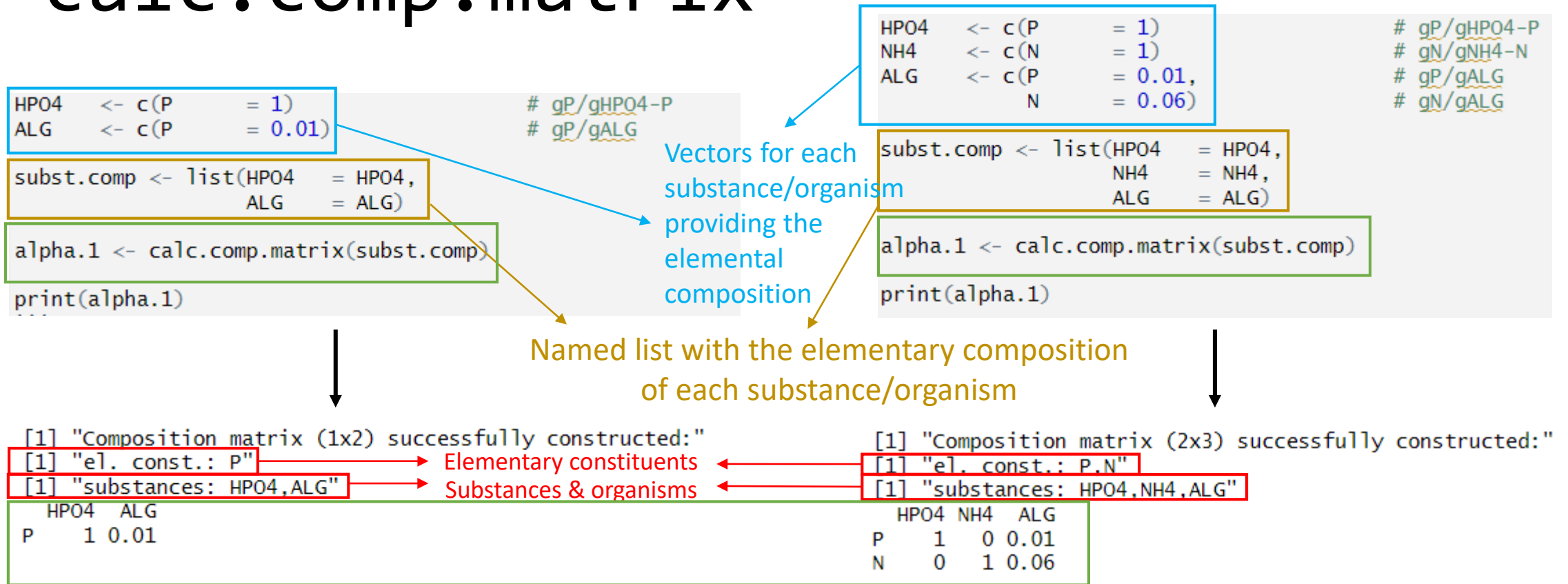
Modelling Aquatic Ecosystems FS24

20.3.2024

# Introduction of the 'stoichcalc' package

- An R package that implements the general solution to calculate stoichiometric coefficients of substances and organisms for different processes.
- The package contains three functions:
  - 'calc.comp.matrix' constructs the **substance composition matrix**
  - 'calc.stoich.coef' calculates the **stoichiometric coefficients**
  - 'calc.stoich.basis' calculates the basis of the **stoichiometry space** (used by the function calc.stoich.coef, not directly in the exercises)
- Using '?stoichcalc' in R for more details.

# 'calc.comp.matrix'



Composition matrix with elementary constituents as rows and substances/organisms as columns

# 'calc.stoich.coef'

```

nu.gro.ALG <-
  calc.stoich.coef(alpha = alpha.1,
                  name   = "growth.ALG",
                  subst  = c("HPO4", "ALG"),
                  subst.norm = "ALG",
                  nu.norm  = 1)

nu.resp.ALG <-
  calc.stoich.coef(alpha = alpha.1,
                  name   = "resp.ALG",
                  subst  = c("HPO4", "ALG"),
                  subst.norm = "ALG",
                  nu.norm  = -1)

nu.1 <- rbind(nu.gro.ALG,
              nu.resp.ALG)

print(nu.1)

```

```

[1] "Number of substances:           2"
[1] "Number of elementary constituents: 1"
[1] "Number of constraints:           0"
[1] "Number of independent processes: 1"
[1] "Stoichiometric coefficients successfully calculated."
[1] "Number of substances:           2"
[1] "Number of elementary constituents: 1"
[1] "Number of constraints:           0"
[1] "Number of independent processes: 1"
[1] "Stoichiometric coefficients successfully calculated."

```

```

      HPO4 ALG
growth.ALG -0.01  1
resp.ALG   0.01 -1

```

- For each process we need to calculate the stoichiometric coefficients separately (growth of algae, respiration of algae .....
- 'alpha' is the composition matrix
- 'subst.norm' is the substance you choose to normalize the stoichiometric coefficients, 'nu.norm' is the value you choose to normalize.

Stoichiometric coefficient matrix nu <sub>4</sub>

Try to do Task 1 in Exercise 3!

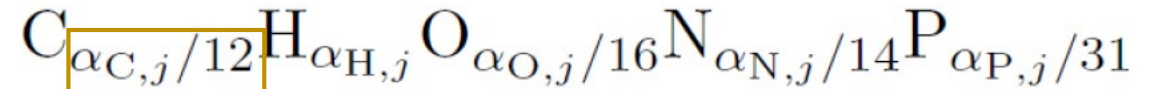
# Stoichiometry of a complex process model

- Parameterized mass fractions (Algae as an example)

Sum of mass fractions [g element per g algae]  
for all elements in a substance/organism should be 1

$$\alpha_{C,j} + \alpha_{H,j} + \alpha_{O,j} + \alpha_{N,j} + \alpha_{P,j} = 1$$

This tells you how many mole of each element  
per gram of algae.



```
param <- list(a.O.ALG = 0.50, # gO/gALG
             a.H.ALG = 0.07, # gH/gALG
             a.N.ALG = 0.06, # gN/gALG
             a.P.ALG = 0.005, # gP/gALG)
param$a.C.ALG = 1 - (param$a.O.ALG + param$a.H.ALG + param$a.N.ALG + param$a.P.ALG)
```

In order to guarantee  
that the fractions sum to 1

```
ALG <- c(C = param$a.C.ALG/12, # molC/gALG
         O = param$a.O.ALG/16, # molO/gALG
         H = param$a.H.ALG,    # molH/gALG
         N = param$a.N.ALG/14, # molN/gALG
         P = param$a.P.ALG/31) # molP/gALG
```

Elemental mass fractions of organisms are  
known according to different compositions. Here  
we use the Redfield composition for algae.

# Stoichiometry of a complex process model

- Constraints  $\gamma$  have to be formulated to fulfill  $\nu_i \cdot (\gamma_{(i)})^T = 0$

We introduce a “yield” for death and adjust it so that neither nutrients nor oxygen are required for dying.

```
param$Y.ALG.death = min(1,param$a.N.ALG/param$a.N.POM,param$a.P.ALG/param$a.P.POM)
param$Y.ZOO.death = min(1,param$a.N.ZOO/param$a.N.POM,param$a.P.ZOO/param$a.P.POM)
```



**$Y_{.death} \leq 1$** , otherwise it means dead particulate organic matter (POM) takes up nutrients from algae or zooplankton. Here we choose it as close to 1 as possible and as small as necessary to avoid negative coefficients for the nutrients.

Constraints provide the relation between two substances/org. We choose one organism to be 1, then the other can be quantified by parameters.

```
nu.gro.ZOO <-
  calc.stoich.coef(alpha      = alpha.2,
                  name       = "gro.ZOO",
                  subst      = c("NH4","HPO4","HCO3","O2","H","H2O","ALG","ZOO","POM"),
                  subst.norm = "ZOO",
                  nu.norm    = 1,
                  constraints = list(c("ZOO" = 1,
                                     "ALG" = param$Y.ZOO),
                                   c("POM" = 1,
                                     "ALG" = param$f.e)))
```

```
[1] "Number of substances:          9"
[1] "Number of elementary constituents: 6"
[1] "Number of constraints:         2"
[1] "Number of independent processes: 1"
[1] "Stoichiometric coefficients successfully calculated."
      NH4 NO3 HPO4 HCO3 O2 H H2O ALG ZOO POM
gro.ZOO 0.011  0   0 0.042 -0.031 0.03 0.011 -5  1  2
```

No. Substances & Organisms = elementary constituents +

No. Constraints +

1 normalized substance/organism

In this example, 9 substances = 6 elements (C,N,P,O,H,charge) + 2 (constraints) + 1 (normalized zooplankton)

Try to do Task 2 in Exercise 3!



# Homework

- Task 3: Homework: Extend the process stoichiometry to sulfur
- Think about theory questions in Exercise 3.

Don't hesitate to ask if you have any questions!

Have a great day!