

Modelling Aquatic Ecosystems

Course 701-0426-00

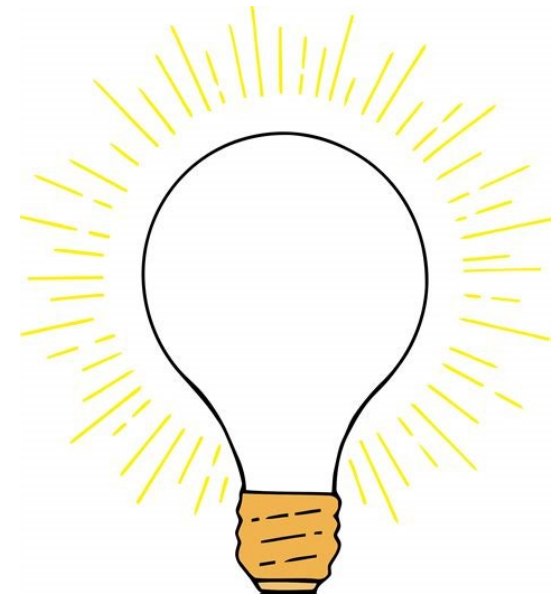
Nele Schuwirth

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Eawag, Swiss Federal Institute of Aquatic Science and Technology

1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
Exercise: R, ecosim-package, simple lake plankton model
Exercise: lake phytoplankton-zooplankton model
2. Process stoichiometry Exercises: analytical solution, calculation with stoichcalc
3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems Exercise: structured, biogeochemical-ecological lake model
Assignments: build your own model by implementing model extensions
5. Physical processes in rivers, bacterial growth, river model for benthic populations Exercise: river model for benthic populations, nutrients and oxygen
6. Stochasticity, uncertainty, Parameter estimation
Exercise: uncertainty, stochasticity
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

- Get a short overview about model structures (chapter 1.3)
- Get short overview about model extensions (chapter 12)
- Get a short overview about research models (chapter 13.1)
- Learn to know some case studies of aquatic ecosystem model applications
- Get hints for the oral exam and clarify open questions
- Feedback about the course

One (big or little) thing
that I learned during this course
that was new to me
and will stick in my head?



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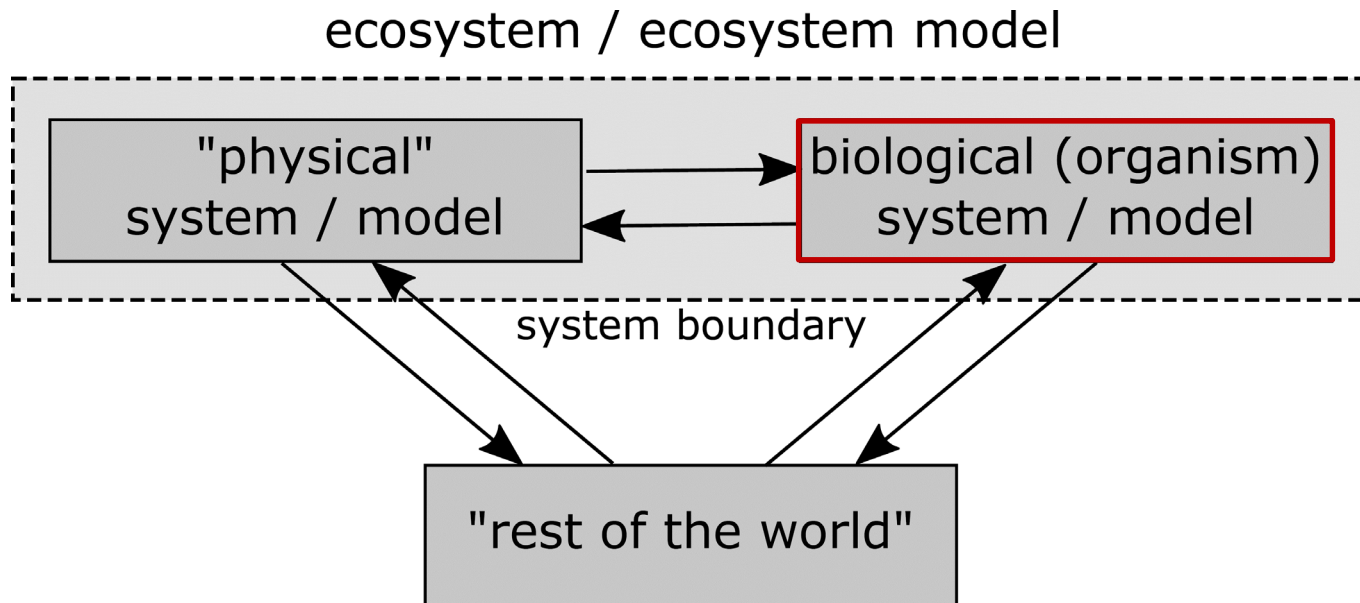


We are really thankful for constructive critique and suggestions for improvement

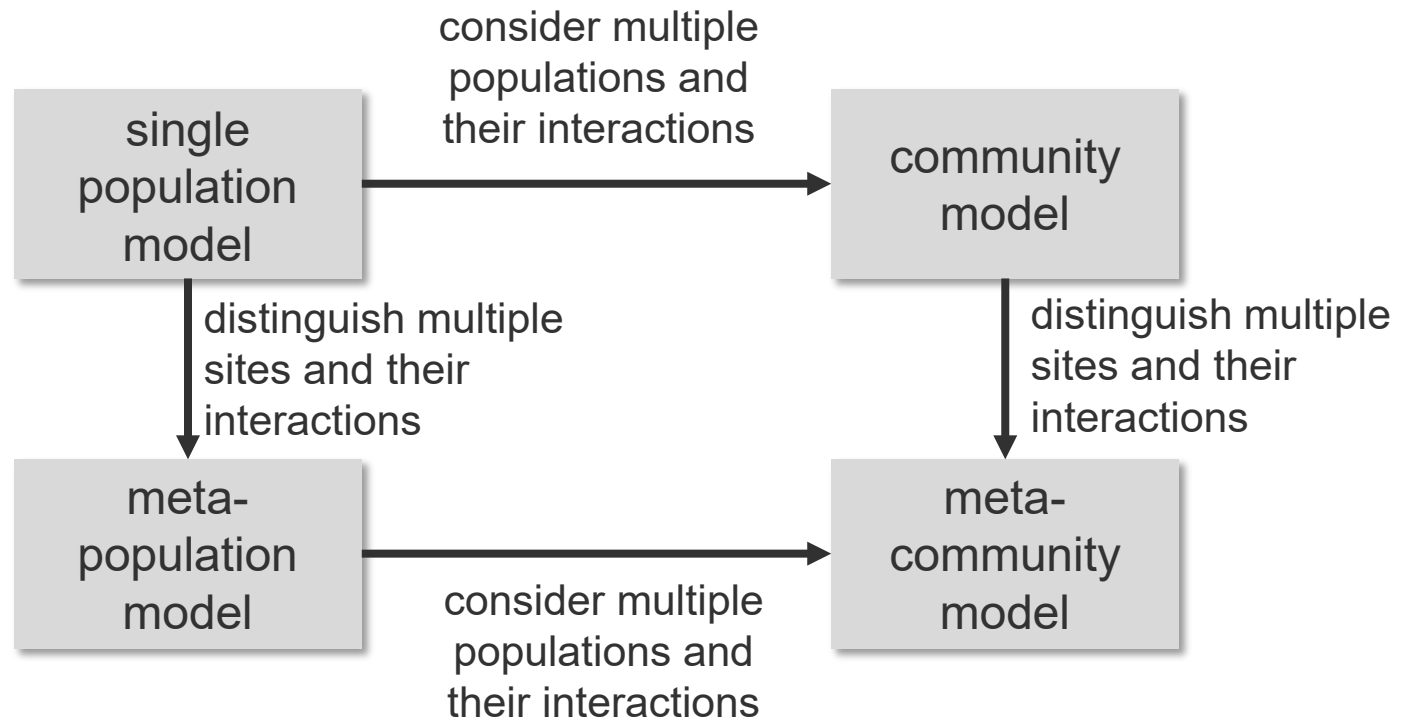
Ecosystem Model

chapter 1.3

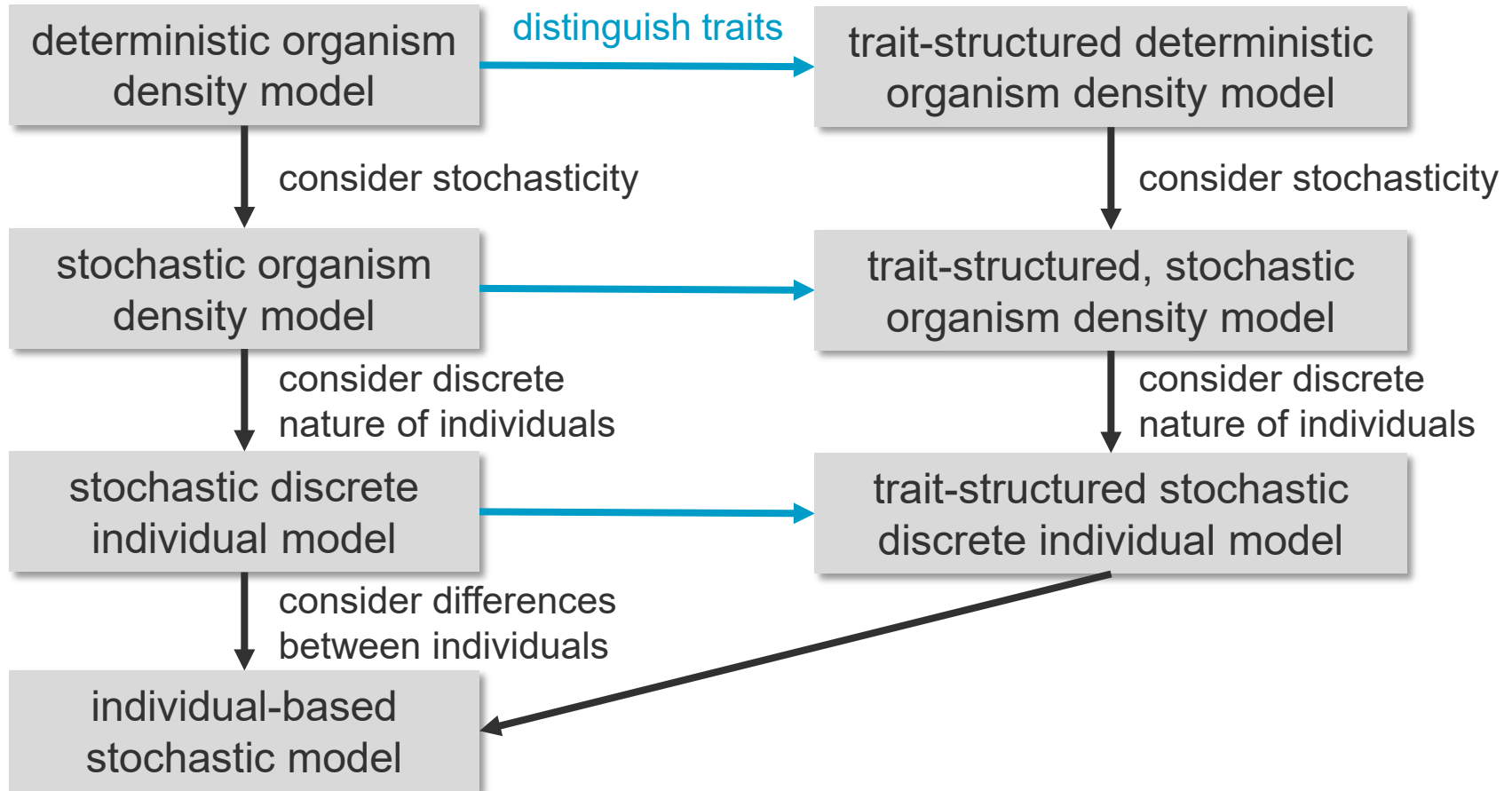
Combines an abiotic, “physical” model and a model of the organisms:



From Populations to Meta-Community Models

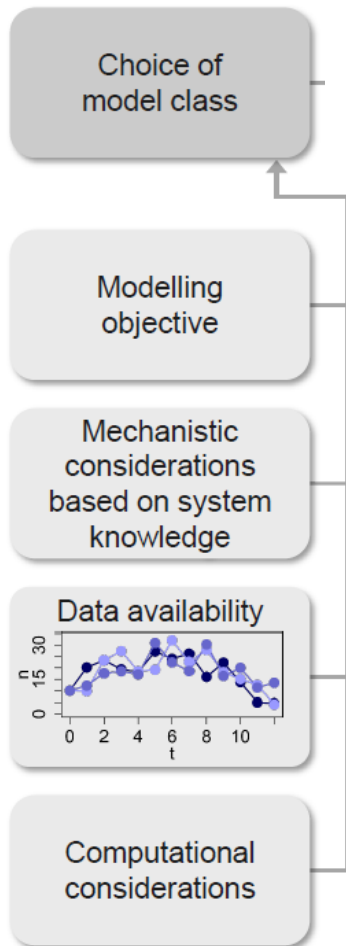


Overview of model classes (for population or community models)

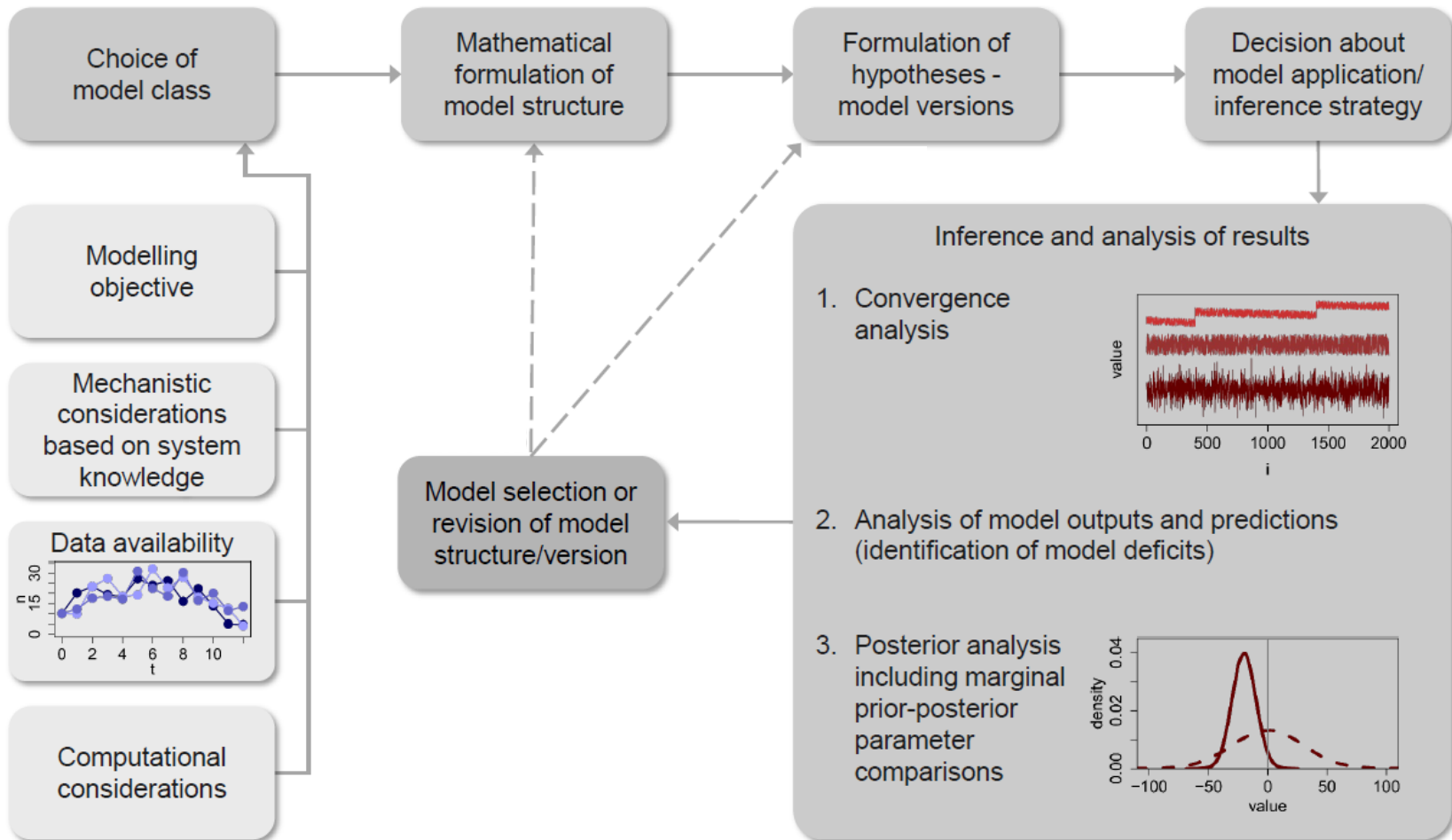


density: e.g. number of organisms per volume, biomass per area

traits: characteristic that distinguishes several groups of organisms



if possible (cross) validation with independent data



if possible (cross) validation with independent data

chapter 12

12.1 Mechanistic description of physical processes

12.2 Important extensions of biological processes

- Diatoms – consideration of silicon
- Variable phosphorus stoichiometry
- Phosphate uptake by organic particles
- Internal concentrations
- **Functional groups**
- **Individual taxa**
- Consideration of rapid evolution

12.3 Important extensions to the model structure

- Age-, size- or stage structured models
- Discrete individuals
- Individual based models

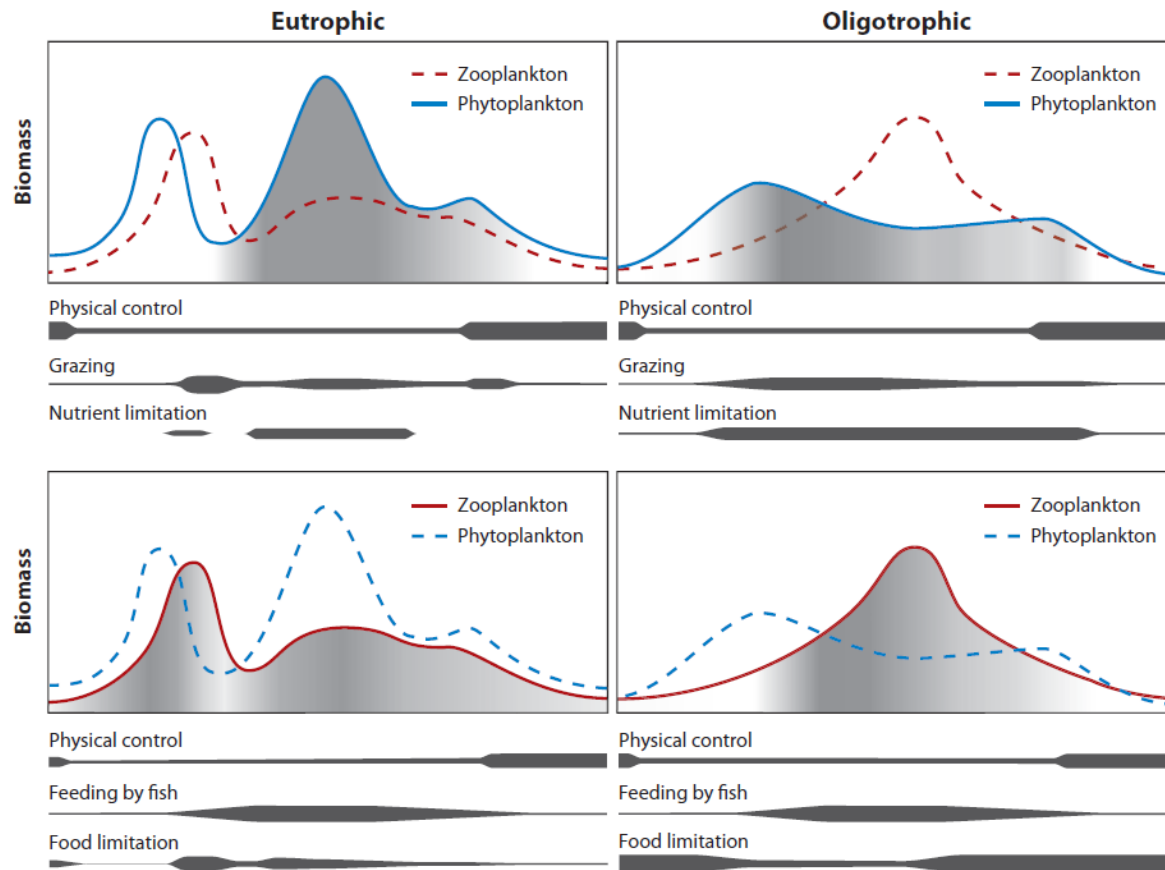
Modelling Functional Groups or Individual Taxa

Functional groups of algae, zooplankton or invertebrates can be distinguished to better account for the diversity of these communities.

Differences for algae could be in

- maximum specific growth rate
- edibility by zooplankton
- sedimentation velocity
- light dependence of growth
- phosphorus dependence of growth
- nitrogen dependence of growth / capability of fixing nitrogen
- silicon dependence of growth

This can lead e.g. to the description of seasonal successions in lake plankton.



Figures 6 and 7 of the original PEG (plankton ecology group) paper (modified): Seasonal (winter through autumn) biomass patterns in eutrophic (left) and oligotrophic (right) water bodies. (Top) Focus on phytoplankton (blue solid line) (dark shading, inedible for zooplankton; light shading, edible for zooplankton). (Bottom) Focus on zooplankton (red solid line) (dark shading, small herbivores; light shading, large herbivores). The thickness of the horizontal bars indicates the seasonal change in relative importance of physical factors, grazing, nutrient limitation, fish predation, and food limitation (with kind permission of E. Schweizerbart publishers).

Modelling Functional Groups or Individual Taxa

When describing individual taxa, the number of parameters becomes overwhelming.

The Metabolic Theory of Ecology (MTE) (Brown et al. 2004) can help to reduce the number of taxon specific parameters. It assumes that the metabolic rates scale with **individual mass M** and **temperature T** :

$$r_{\text{basal}} = i_0 \left(\frac{M}{M_0} \right)^b \exp \left(-\frac{E_a}{k_B} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right)$$

i_0 normalization constant

M individual body mass

b scaling exponent

E_a activation energy (eV)

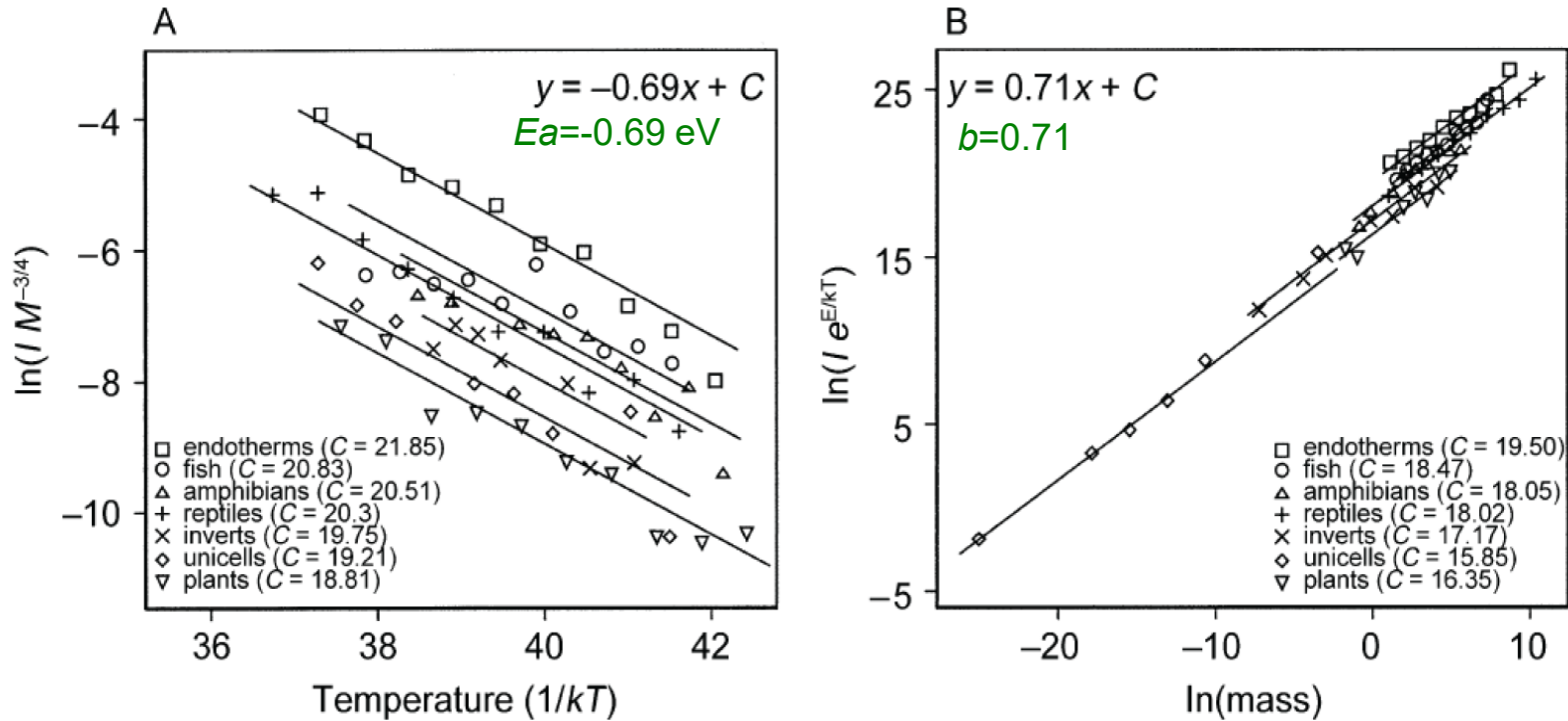
k_B Boltzmann's constant

T absolute temperature in K

The parameters in **green** can be derived from experiments universally for all organisms or for groups of organisms at coarser taxonomic levels.

Modelling Functional Groups or Individual Taxa

The parameters in green can be derived from experiments universally or for groups of organisms at coarser taxonomic levels.



(from Brown et al. 2004 after Gillooly et al. 2001)

Modelling Functional Groups or Individual Taxa

Growth, respiration, and death rates are found to be multiples of the basal metabolic rate

Temperature-corrected maximum production rates [g/ind/year]

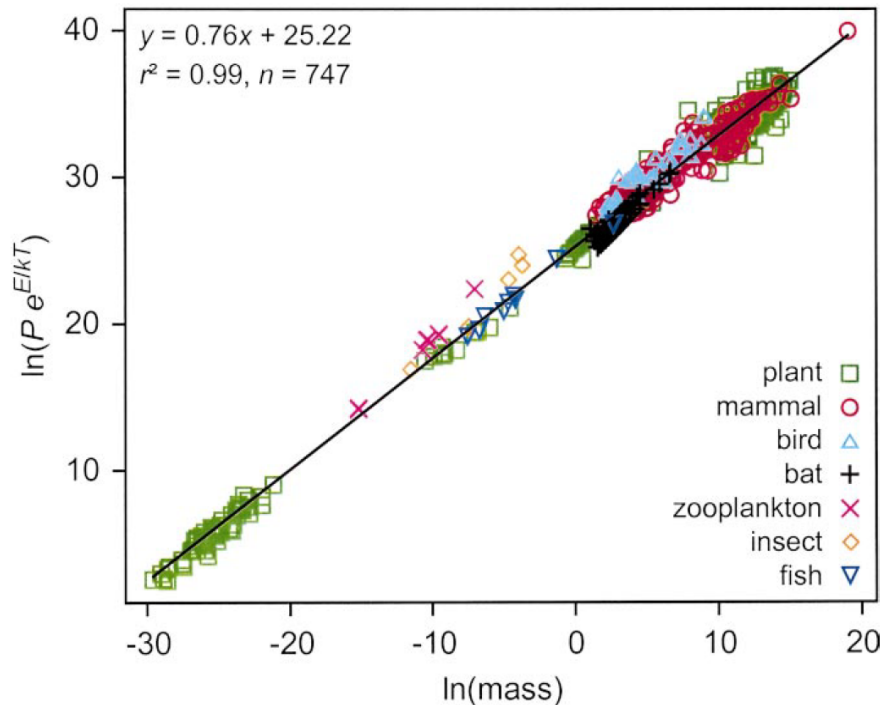


FIG. 2. Mass dependence (mass measured in grams) of temperature-corrected maximal rates of whole-organism biomass production ($Pe^{E/kT}$, measured in grams per individual per year) for a wide variety of organisms, from unicellular eukaryotes to plants and mammals (from Ernest et al. 2003). Data, which span >20 orders of magnitude in body size, have been temperature corrected using Eq. 6. The allometric exponent, indicated by the slope, is close to the predicted value of $\frac{3}{4}$ (95% CI, 0.75–0.76).

Brown et al. 2004
from Ernest et al. 2003

Lake Models / Simulation Programs

- BELAMO
- SALMO
- CAEDYM
- PCLake+
- AQUATOX
- CASM
- StoLaM+StreamCom

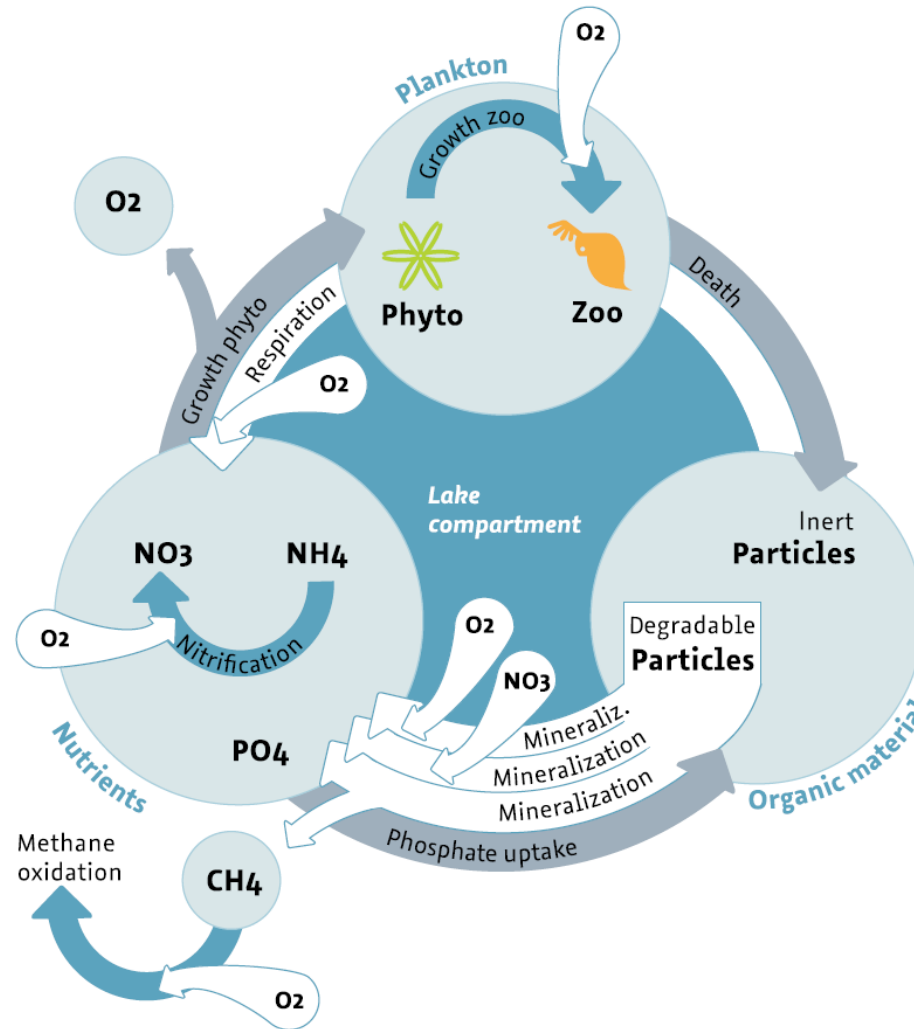
River Models / Simulation Programs

- QUAL2K
- RWQM1
- ERIMO
- Streambugs

see Janssen et al. 2015: "Exploring, exploiting and evolving diversity of aquatic ecosystem models: a community perspective". *Aquatic Ecology* **49**:513-548 for a recent review [link](https://link.springer.com/article/10.1007/s10452-015-9544-1)

<https://link.springer.com/article/10.1007/s10452-015-9544-1>

BELAMO: Biogeochemical-Ecological Lake Model - applied to Swiss lakes



BELAMO, Model Assumptions:

- Continuous resolution of the vertical dimension, distinction of water column and two sediment layers.
- Variables: NH_4^+ , NO_3^- , HPO_4^{2-} , O_2 , ALG, PLR, ZOO.
- Processes: Growth, respiration and death of ALG, PLR (*Planktothrix rubescens*) and ZOO; aerobic and anoxic mineralization; nitrification; P-uptake of sedimenting particles.
- Variable composition/stoichiometry with respect to P.

BELAMO: Biogeochemical-Ecological Lake Model - applied to Swiss lakes

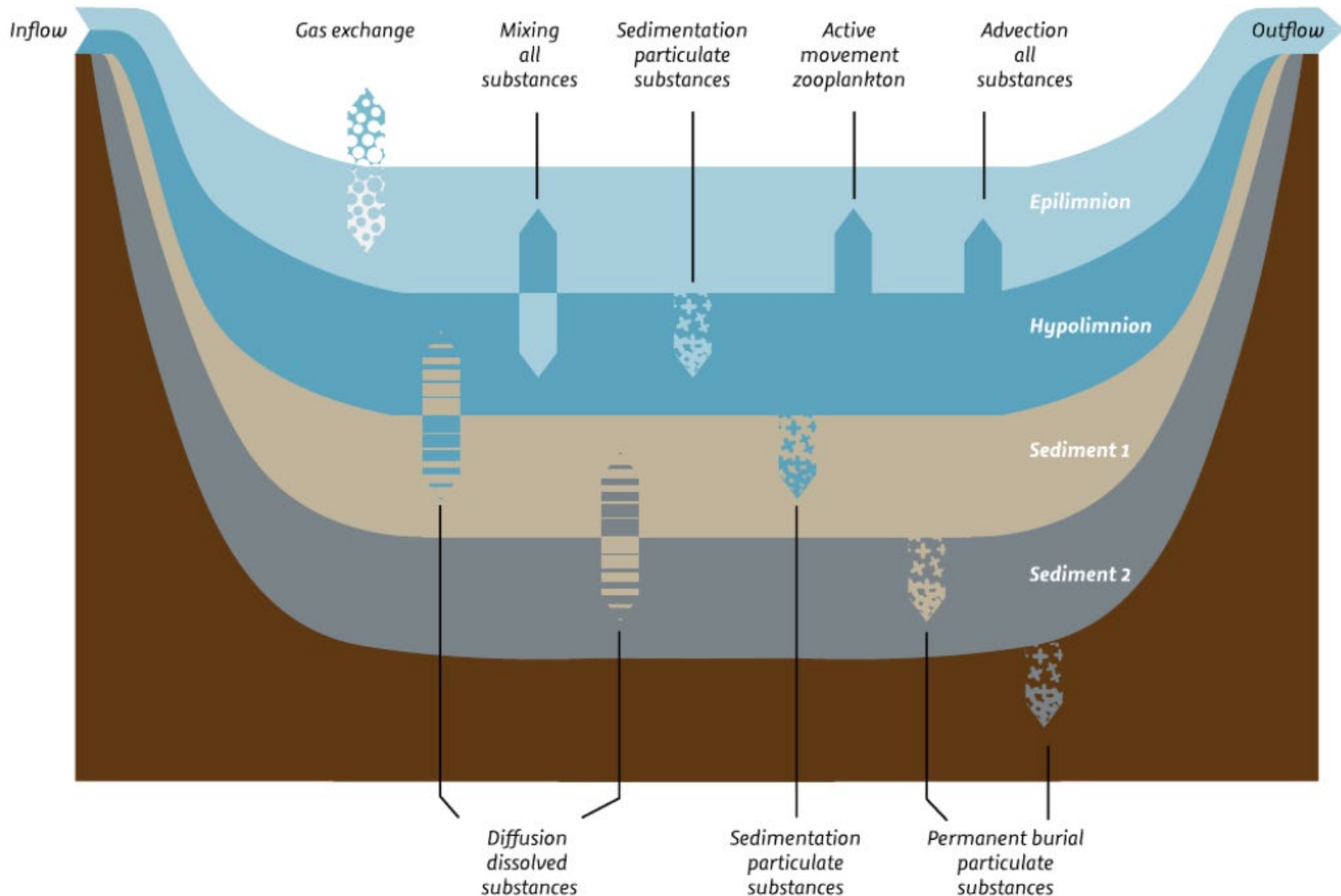
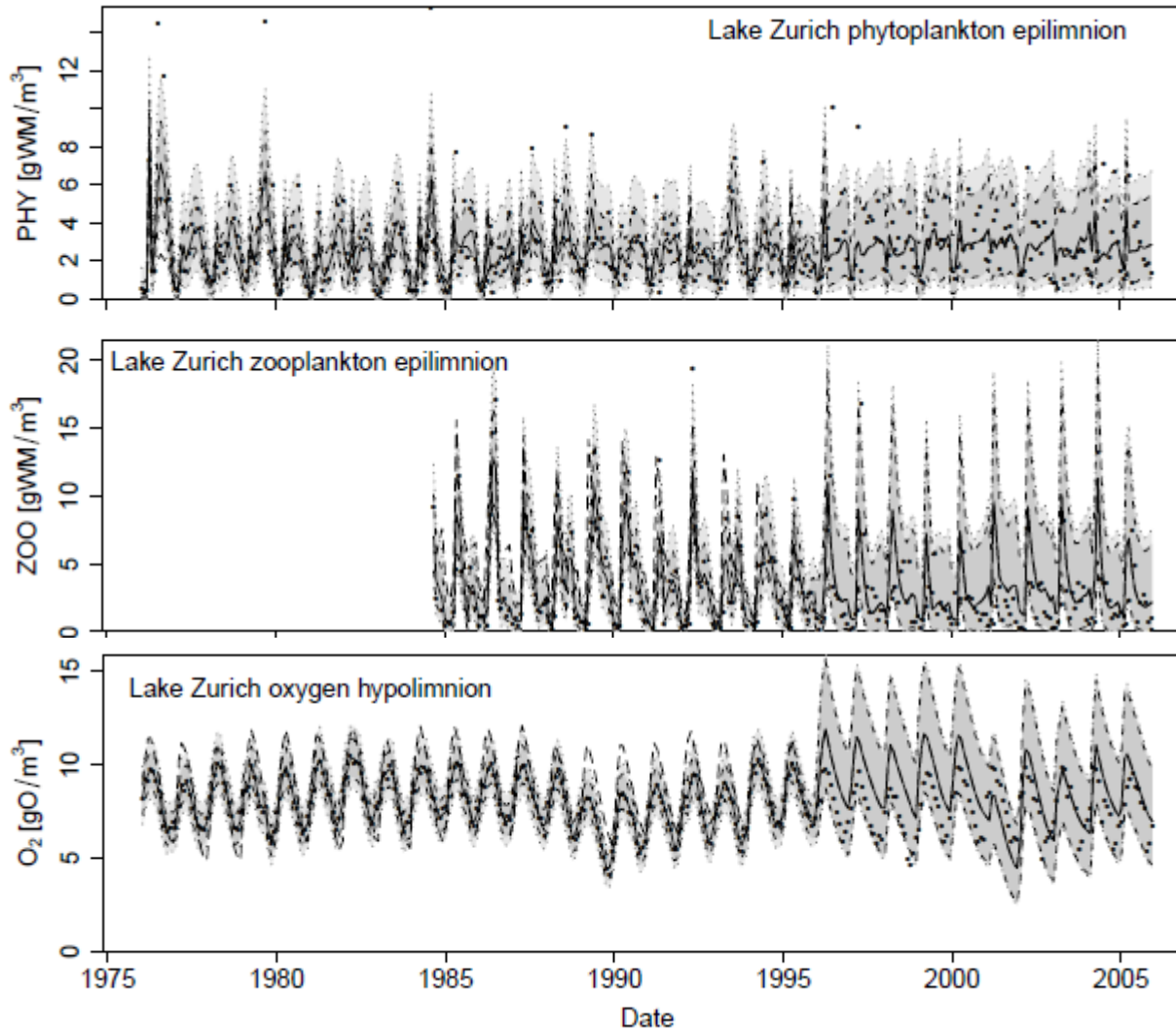
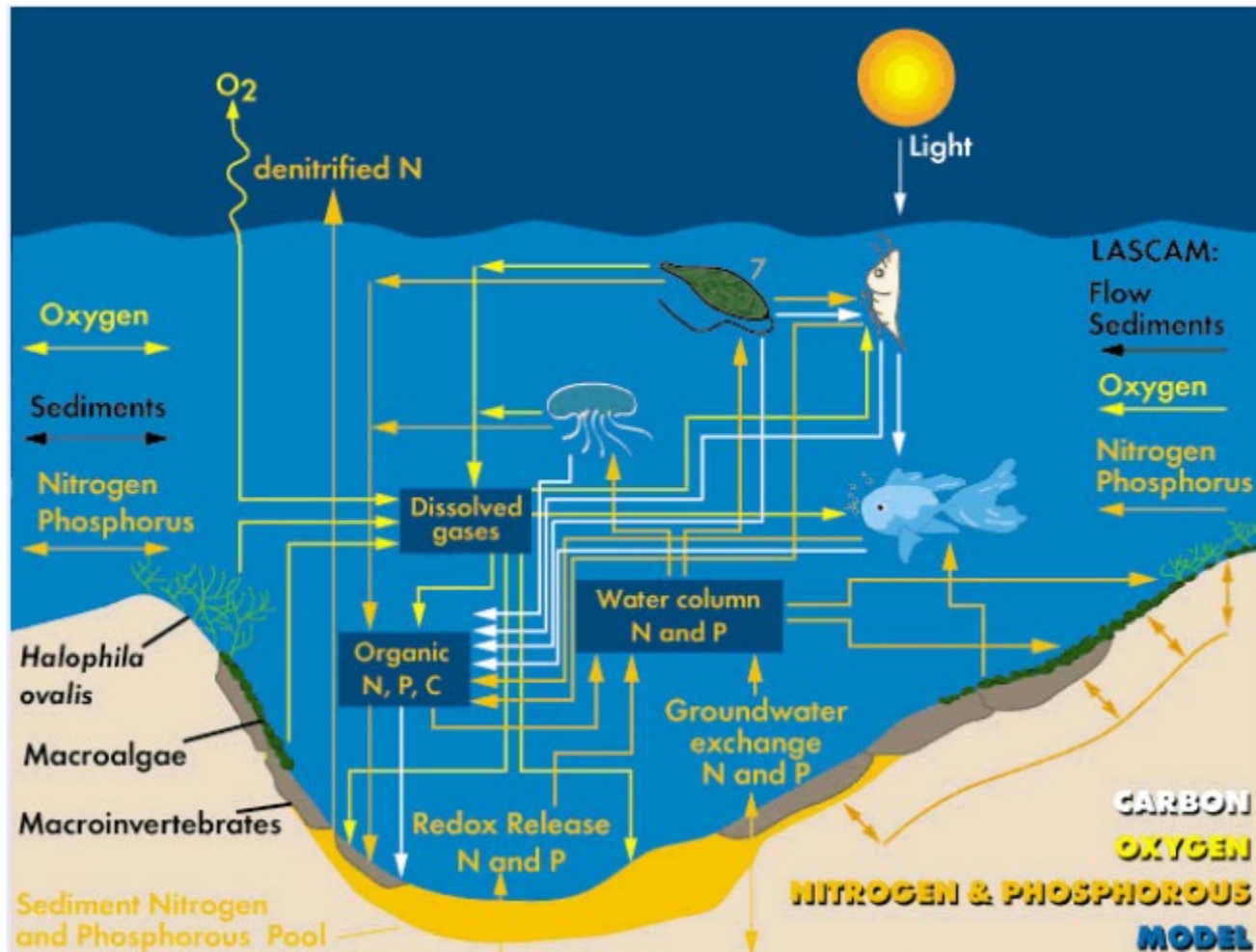


Fig. 2 Structure and physical processes of the four-box version of BELAMO.

BELAMO: Biogeochemical-Ecological Lake Model - applied to Swiss lakes

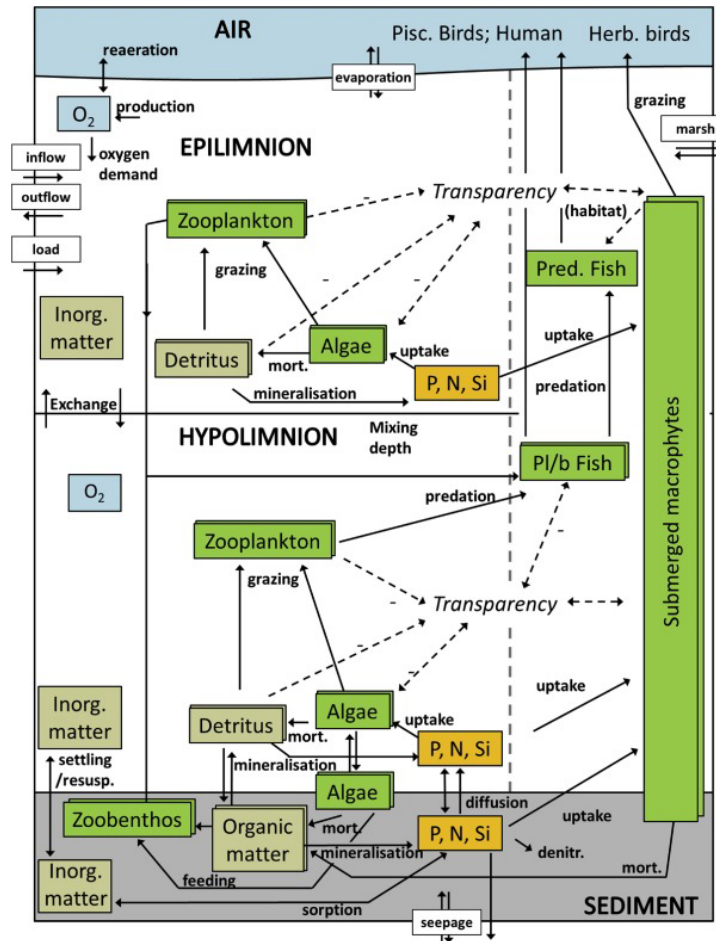


CAEDYM: Computational Aquatic Ecosystem Dynamics Model

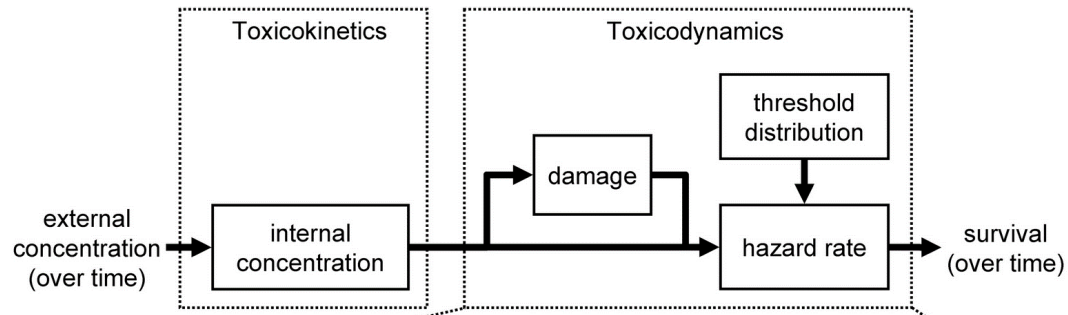


<http://www.cwr.uwa.edu.au/software1/models1.php?mdid=3>

PCLake+: A process-based ecological model to assess the trophic state of stratified and non-stratified freshwater lakes worldwide

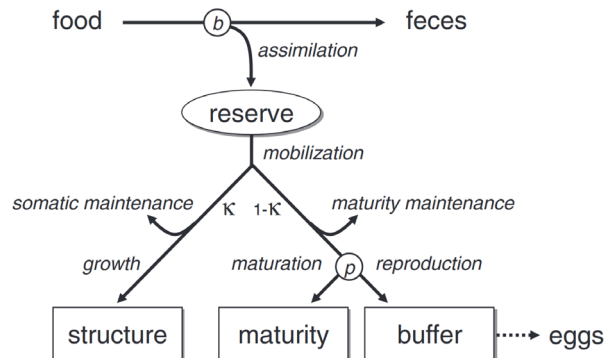


- Survival model for toxic effects: Toxicokinetic-toxicodynamic models TK/TD e.g. General Unified Threshold model for Survival GUTS



from Jager et al. *Environ. Sci. Technol.* 2011, 45, 7, 2529-2540

- Dynamic Energy Budget model with toxic effects: DEBtox (www.debtox.info/)



T. Jager, H. Selck / *Journal of Sea Research* 66 (2011) 456–462

Original DEB theory: Kooijmann 2001 *Phil. Trans.R.Soc.Lond. B* 30

Examples from current research:
Streambugs:
**A mechanistic model for the community
composition of macroinvertebrates in streams**



Motivation

- test our **understanding** of **ecosystem functioning**
- identify influential sources of **human disturbance**
- predict consequences of **management** options
(river restoration, upgrade of waste water treatment plants, risk assessment of pesticides with mesocosm experiments)
- assess impact of **future development** (climate change, land use)



Why macroinvertebrates?

- functional role in stream ecosystems
- important part of biodiversity in stream ecosystems
- indicators for the ecological status of streams

→ Linking functional and structural aspects of the ecosystem



Streambugs Concept

- formulate dynamic food web model with ordinary differential equations based on **mass balances**
- use **stoichiometry** to bound yields and link between the benthos community and biogeochemical cycles
- use allometric scaling to reduce number of parameters and fits of the **Metabolic Theory of Ecology** to measured data to estimate "universal" parameters for basal metabolism used to scale all biological rates
- modify rates based on autecological **trait information** and environmental conditions
- propagate parameter and input **uncertainty**
- Bayesian inference to learn about the parameters from observed data and reduce model output uncertainty

Implementation as R-package "streambugs" and new Julia version in development

Streambugs Process Table

Processes	State variables						
	Periphyton (g DM)	Invert. taxa (g DM)	Litter (g DM)	FPOM (g DM)	Food (g DM)	Nutrients	Oxygen
pp gro	1					-	+
pp resp	-1					+	-
pp mort	-1			$+Y_{\text{mort}}$		+/0	+/0
cons gro		+1		$+f_e/Y_{\text{gro}}$	$-1/Y_{\text{gro}}$	+/0	+/-
cons resp		-1				+	-
cons mort		-1		$+Y_{\text{mort}}$		+/0	+/0
Litter inp			+1				

Processes: **growth, respiration, and mortality** of primary producers (pp) and consumers (cons), leaf litter input

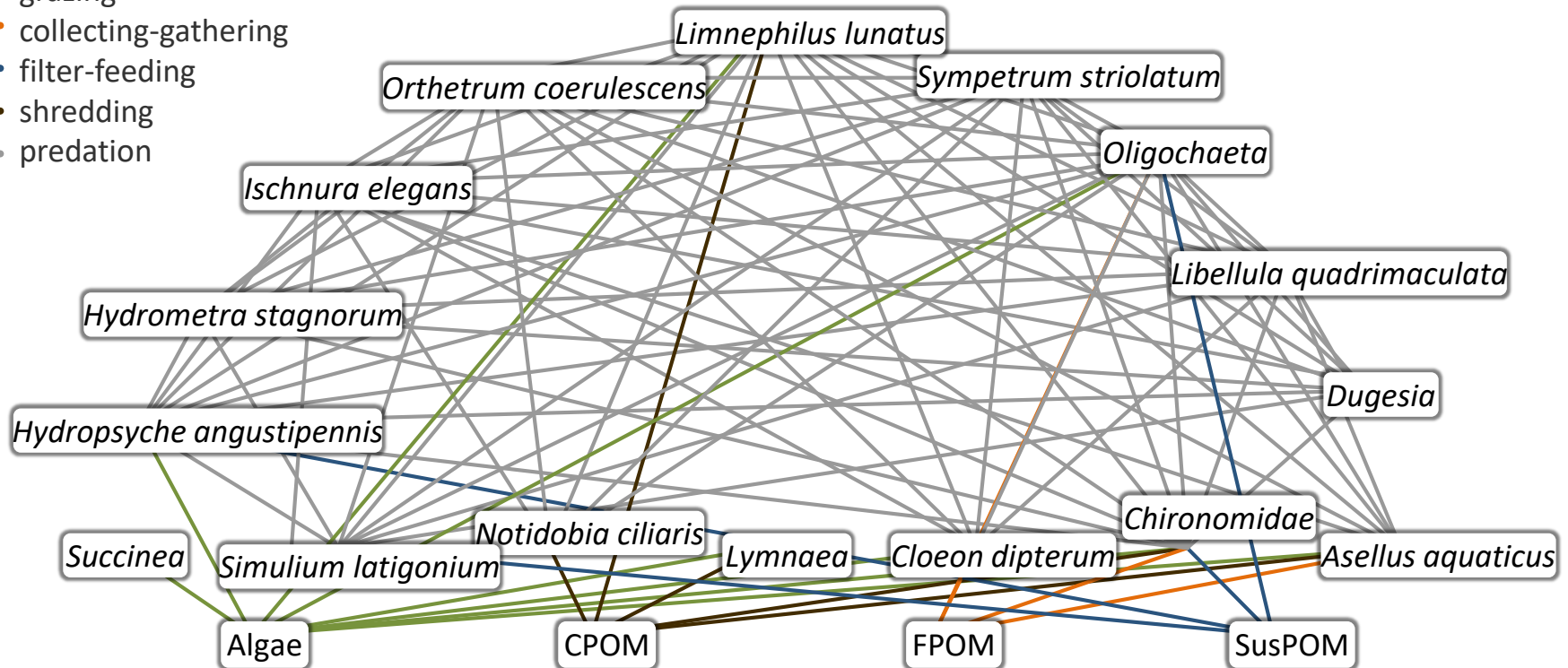
pp: two types of periphyton (filamentous algae and crusty algae)

cons: different macroinvertebrate taxa

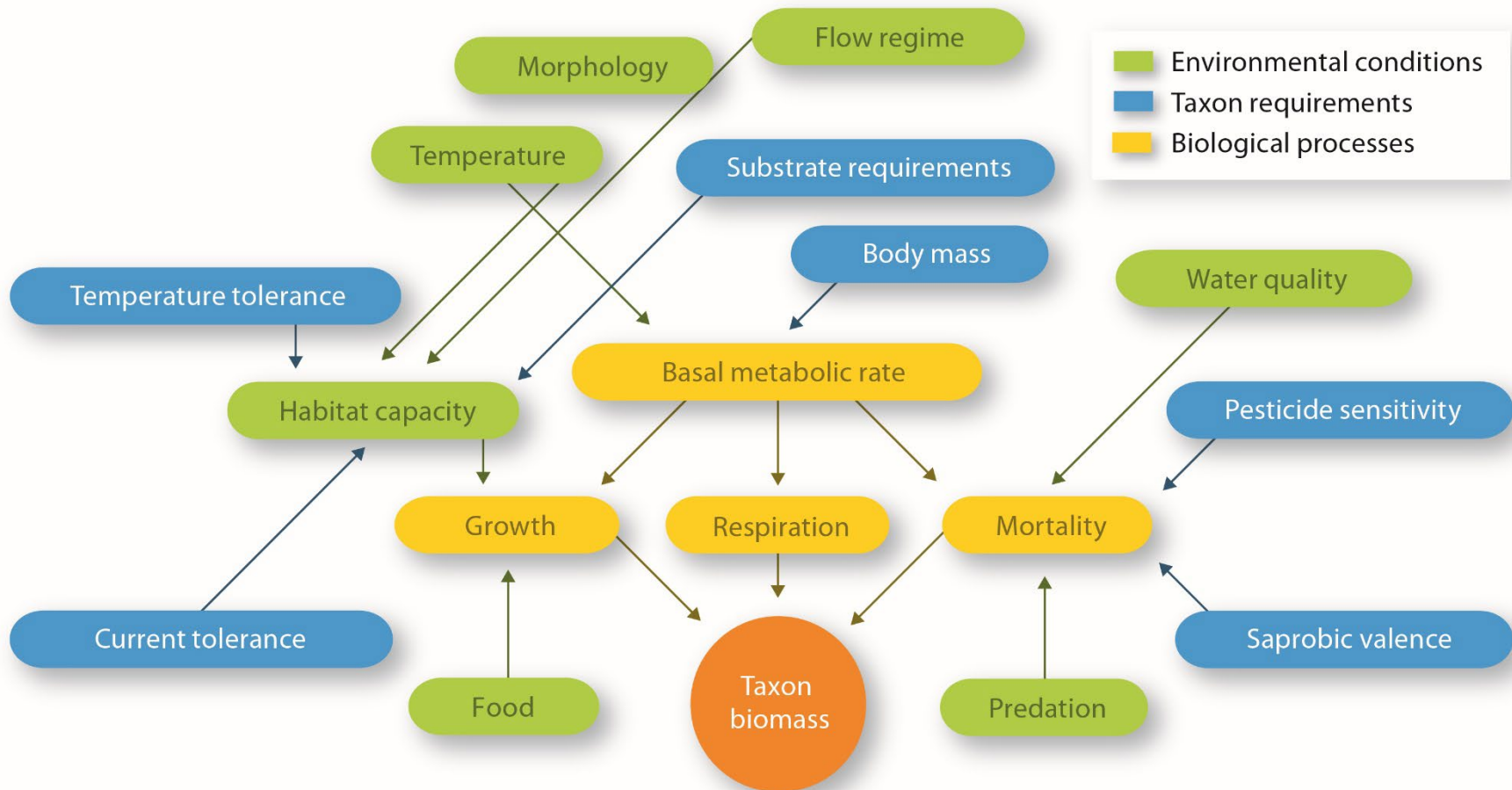
Streambugs: Food web

feeding links

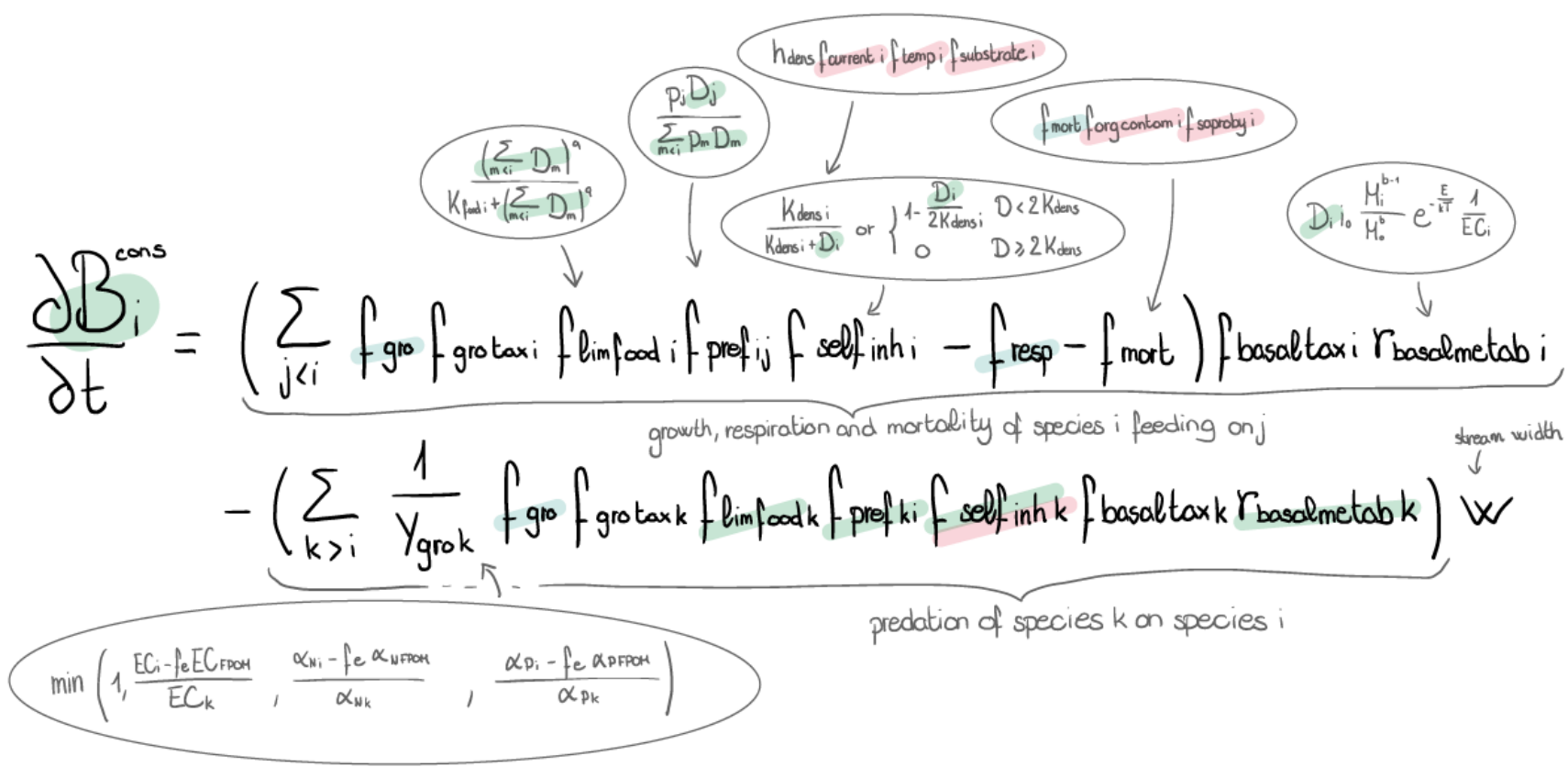
- grazing
- collecting-gathering
- filter-feeding
- shredding
- predation



Streambugs



Streambugs



= state variables,
 = env. conditions preferences,
 = universal (species independent)

Streambugs

Modelling **temporal biomass dynamics** of invertebrate communities

- in stream **mesocosms** contaminated with a **pesticide** (Thiacloprid)
Kattwinkel et al. 2016 *ES&T*
- in a Swiss **river** during **hydropeaking** experiments
Mondy & Schuwirth 2017 *Ecol. Appl.*
- in pond mesocosms contaminated with pesticides for registration
(ongoing collaboration with industry partners)

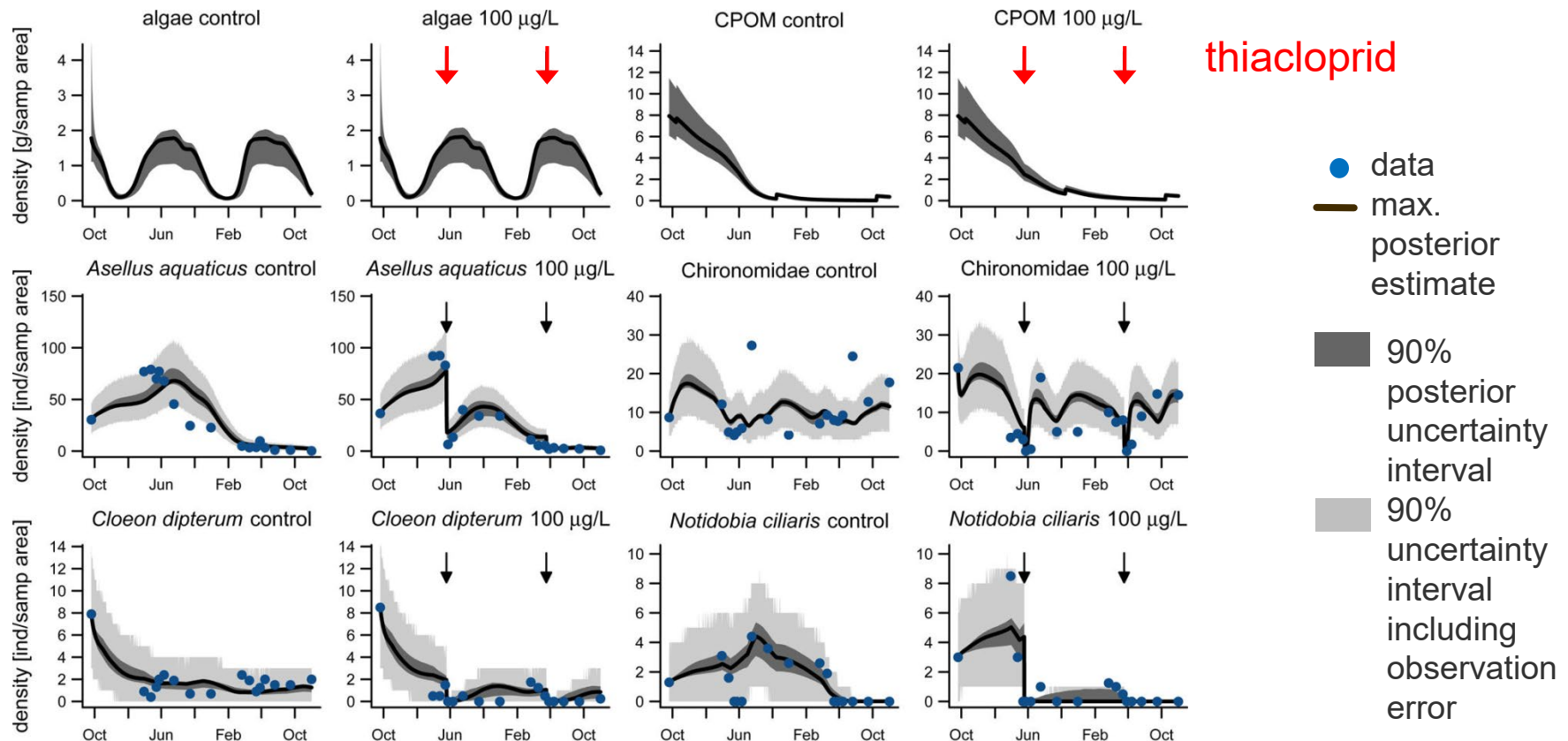


Modelling the probability of **occurrence** of invertebrates

- to predict effects of **river restoration** in two Swiss **rivers**
Paillex et al. 2017 *FWB*
- **in a catchment** at the Swiss Plateau to assess the importance of biotic interactions and **multiple stressors**
Schuwirth, Dietzel, Reichert 2016 *Functional Ecol.*



Case Study 1: Community dynamics in mesocosms





Hints for the oral examination of the course "Modelling aquatic ecosystems"

Main goals of the course: The students are able to:

- build mathematical models of aquatic ecosystems that consider the most important physical, chemical, biogeochemical, biological, and ecological processes
- explain the interactions between these processes, especially between ecological and biogeochemical processes, and the behaviour of the system that results from these interacting processes based on a model they developed themselves
- formulate, implement and apply simple ecological models
- describe the main sources of uncertainty and key concepts of parameter estimation

The oral exams are aligned with these objectives. However, the technical model implementation with R is not part of the examination.

Important aspects of the exams are:

1. Formulation of mass balance equations and transformation processes; consideration of conservation laws for elements and charge for the formulation of biological and chemical transformation processes, parameterization of process rates, process table notation, important processes in aquatic ecosystems (lakes and rivers)
2. Qualitative behaviour of model solutions; how model outputs change due to changes in parameter values or external influence factors; important interactions in model outputs (interdependencies between state variables), dominant mass fluxes in the models (and the systems described by the models)
3. Important sources for uncertainty in model outputs; how they can be considered in the model.

Prerequisite for participating in the oral exam is that the student has submitted their model assignment (see program, submission deadline is 24.05.2024).

Half of the time of the oral exam will be devoted to discussing the results of the model assignments. The other half will cover other course topics.

Minimum requirement for passing is that the student can correctly describe how to derive the stoichiometric coefficients and how to formulate the transformation rate for a given biological process.

The oral exams will take place on 07./10./11. of June 2024 at Eawag, Dübendorf. The exams take 30 minutes and will be graded.

Typical example questions can be found on the next page.

Typical examples for examination questions

Explain the model that you have developed during the course. What were the most important changes compared to the model 11.4? Please describe the temporal development of the state variables. Explain the results of your sensitivity analysis.

Explain the process table notation using a simple lake model as an example.

For a simple one box model, explain how to derive the differential equations based on the process table.

How can you calculate the total net transformation rate for a single substance, which is involved in several transformation processes?

Given a biological process x (from those described in chapter 8), explain what is happening in this process. How can you derive the stoichiometric coefficients for this process? How can you find out, if additional constraints are needed?

Which are drawbacks of the simplified approach to address this question?

How can you avoid additional manual calculations to derive the stoichiometric coefficients, if the composition of a substance changes?

How can you formulate the additional stoichiometric constraints that are needed for the growth of secondary producers (e.g. zooplankton)?

When do you need to introduce a yield for the death process of algae and zooplankton?

What would be an alternative solution to the introduction of such a yield?

Given the biological process x , how can you formulate the process rate?

What are the typical elements for process rates of biological processes?

How can you decide for which substances in the process rate a limitation term is needed?

Which alternatives may be used to formulate the limitation and inhibition terms?

Sketch the food web of the benthic (pelagic) zone of a river (lake).

Which transformation processes have to be considered in a lake model to describe the phosphorus (nitrogen) cycle?

What are important transport processes that have to be considered in a lake model?

What are important transport processes that have to be considered in a river model?

What must be considered when discretizing a river model as a system of mixed reactors?

What influences the flow velocity in a river? What influences the water depth in a river?

Which processes affect the oxygen concentration in a river/lake?

Which alternatives do you know to model the mineralisation of organic material in aquatic ecosystems?

Which alternatives do you know to model nitrification in aquatic ecosystems?

How can you assess the sensitivity of a model to single parameters in a simple way?

What are important sources of model uncertainty? How can they be considered in a model?

How can you obtain the values for the model parameters?

How can you use observed data to improve your parameter estimates?

Other examples are the questions from the exercises.

You are able to:

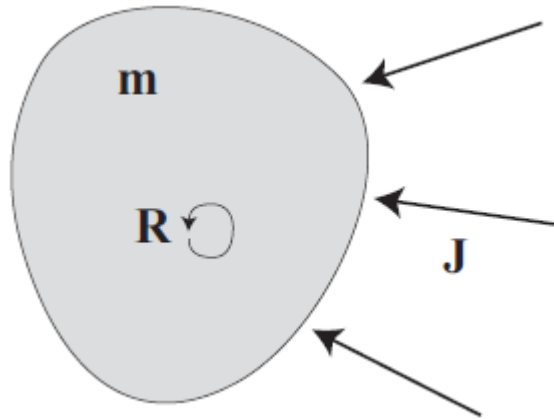
- build mathematical models of aquatic ecosystems that consider the most important biological, biogeochemical and physical processes
- explain the interactions between these processes and the behaviour of the system that results from these interacting processes
- formulate, implement and apply simple ecological models
- describe the main sources of uncertainty and key concepts of parameter estimation

The oral exams are aligned with these objectives. However, the technical model implementation with R is not part of the examination.

- Be precise with the use of terms (e.g. state variable, process rate, rate constant, stoichiometric coefficient, parameter) and aware about units/dimensions
- Be able to explain the process table notation and how to derive the differential equations from it for a simple box model
- Be ready to write down a qualitative process table for a given biological process and explain how to derive the stoichiometric coefficients
- Be ready to explain the typical elements of process rates and to give a concrete example for the different terms for a given biological process
- Be able to explain what the most important physical transport processes are for lake and river ecosystems (we don't ask about the concrete equations but e.g. which factors affect the flow velocity in a river)

+ know about your model assignment!

General Principles and One Box Model



integral form:

$$m(t_{\text{end}}) = m(t_{\text{ini}}) + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{J}(t) dt + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{R}(t) dt$$

differential form:

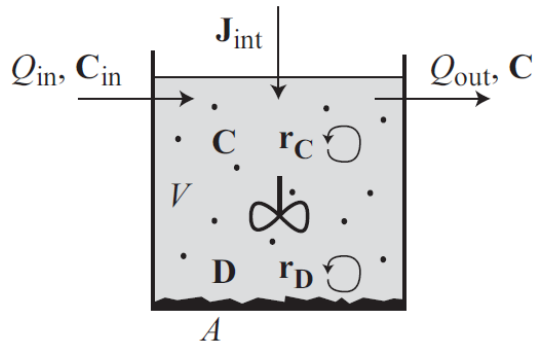
$$\frac{dm}{dt}(t) = \mathbf{J}(t) + \mathbf{R}(t)$$

volume change as difference of inflow - outflow

inflow - outflow caused by water flow

mass flow across interfaces not related to water flow (e.g. sedimentation, gas exchange)

special case: one box



$$\frac{dV}{dt} = Q_{\text{in}} - Q_{\text{out}}$$

$$\frac{dC}{dt} = \frac{Q_{\text{in}}}{V} (C_{\text{in}} - C) + \frac{J_{\text{int}}}{V} + r_C$$

$$\frac{dD}{dt} = r_D$$

effect of transformation processes

Process	Substances					Rate
	s_1	s_2	s_3	\dots	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	\dots	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	\dots	ν_{2n_s}	ρ_2
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
p_{n_p}	$\nu_{n_p 1}$	$\nu_{n_p 2}$	$\nu_{n_p 3}$	\dots	$\nu_{n_p n_s}$	ρ_{n_p}

Substance transformation rate in homogeneous environment:

$$r_j = \sum_{i=1}^{n_p} \nu_{ij} \rho_i$$

One of the (non-zero) stoichiometric coefficients, ν_{ij} , in each row can be selected to be plus or minus unity. This makes the corresponding process rate, ρ_j , to the (positive or negative) contribution of this process to the total transformation rate of the corresponding substance, s_i .

3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution

be able to explain how to do this for a given biological process (from chapter 8)

rate
parameter
under
standard
conditions

temperature
dependence

dependence on
other env. factors,
here light

$$\rho_{\text{gro,ALG,NH}_4^+} = k_{\text{gro,ALG},T_0} \cdot f_{\text{temp}}(T) \cdot f_{\text{rad}}(I) \cdot \underbrace{f_{\text{lim}}(C_{\text{HPO}_4^{2-}}, C_{\text{NH}_4^+}, C_{\text{NO}_3^-})}_{\text{limitation terms for all "substances" that have a negative stoich. coefficient}} \cdot \underbrace{C_{\text{ALG}}}_{\text{dependence on the concentration of the substance to which the stoichiometry was normalized}}$$

limitation terms for all "substances"
that have a negative stoich. coefficient

+ maybe inhibition terms

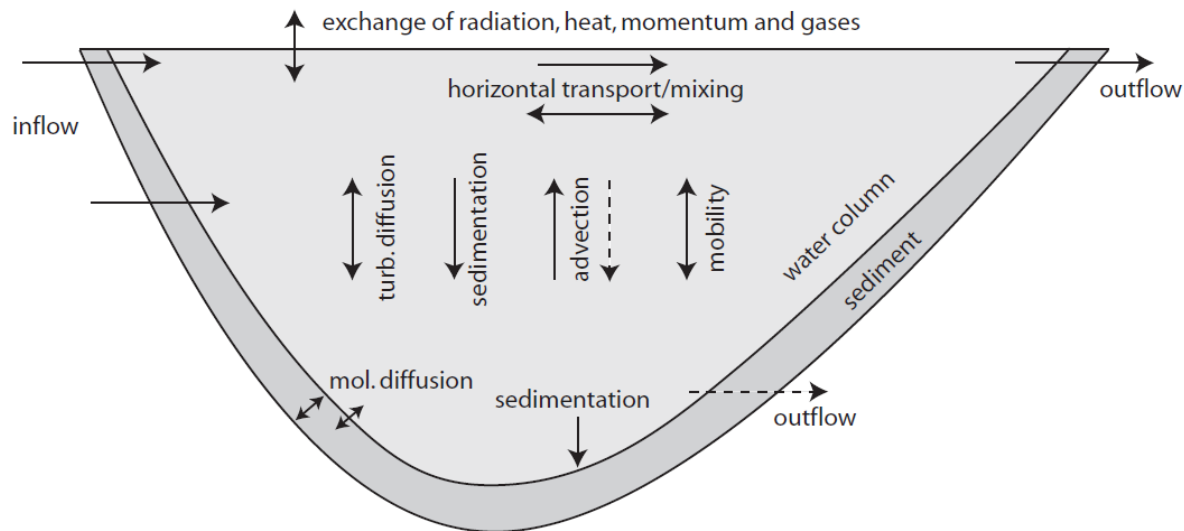
dependence on the
concentration of the
substance to which
the stoichiometry
was normalized

be able to give a concrete example for the f's

Mathematical formulation of biological processes, in particular

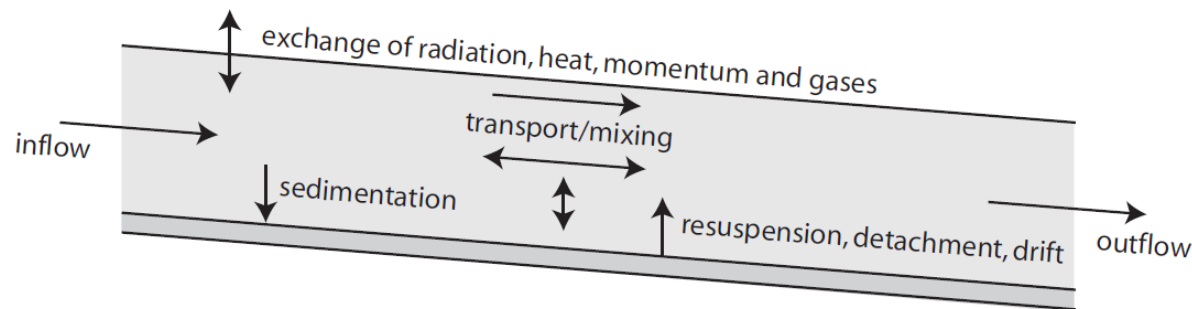
- primary production (e.g. growth of algae)
- respiration
- death
- consumption (e.g. growth of zooplankton)
- mineralization (aerobic, anaerobic, anoxic)
- nitrification (one or two step process)
- growth of heterotrophic bacteria
- growth of nitrifying bacteria

- Advection:** Transport of a substance by directed bulk motion of a fluid, in our case transport with water flow.
- Sedimentation:** Directed transport of particles in a fluid (water) caused by gravitational forces rather than by water flow.
- Diffusion:** Undirected transport (mixing) due to molecular motion (**molecular diffusion**) or turbulent eddies (**turbulent diffusion**).
- Dispersion:** Mixing in flow direction due to transverse diffusion of particles between flow with different advective velocity (“shear flow dispersion”, see transport and mixing in rivers).



Overview of substance transport and mixing processes in rivers under steady-state hydraulic conditions:

- the estimation of average flow velocity and water depth
- vertical mixing
- lateral mixing
- longitudinal transport and dispersion

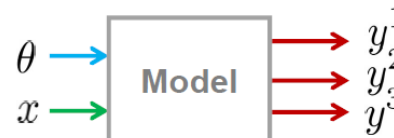
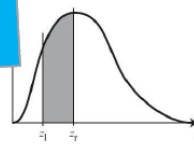


Model uncertainties

1. Input uncertainty
2. Parameter uncertainty
3. Model structure uncertainty
4. Output (measurement) uncertainty
5. (Scenario uncertainty)

Stop worrying and use
Monte Carlo error propagation!

Uncertainties can be described by
probability distributions



Parameter values

Information sources:



i) literature

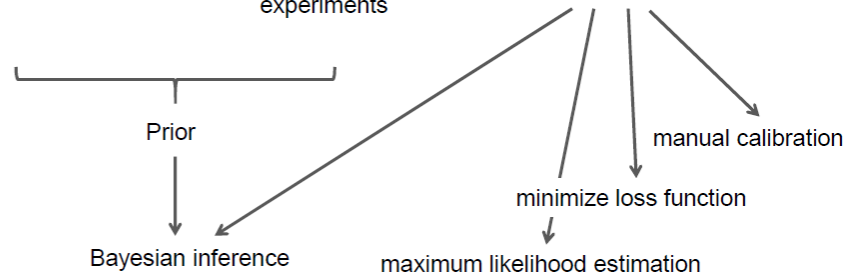


ii) laboratory
experiments



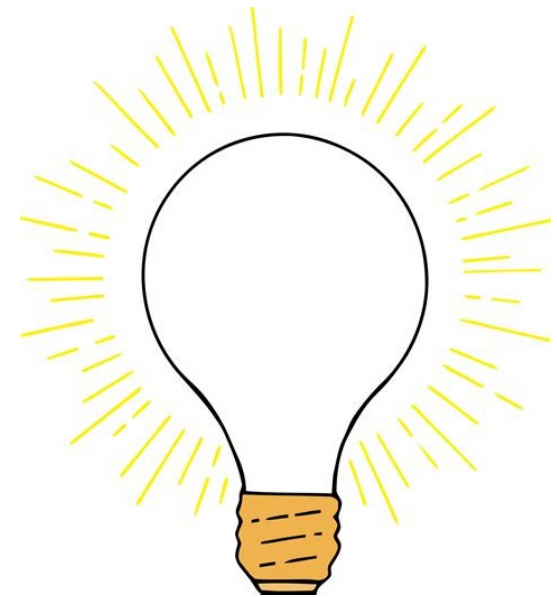
iii) field measurements

Model calibration:



Last Chance for Questions

One (big or little) thing
that I learned during this course
that was new to me
and will stick in my head?



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A big thanks to all contributors!



Emma Chollet Ramampandra



Chuxinyao (Nick) Wang



Andreas Scheidegger



Peter Reichert

and you for your active participation!

Prepare well!

Stay calm!

Good luck!

Thanks for your participation
and all the best for your future!