Process-based Aquatic Ecosystem Modeling

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = q_0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\nabla\mathbf{v} = -\frac{1}{p}\nabla p + g + \nu\Delta\mathbf{v}$$

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UNIVERSITY OF WISCONSIN–MADISON
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NSF

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Process-based Aquatic Ecosystem Modeling
(GLM-AED2 in R)

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supported by NSF ABI development grant, #DBI 1759865

Who’s who?

Robert, postdoc at
UW-Madison
modeling enthusiast

#carbon

Austin, grad
student at
UW-Madison

**guest talk by DIY
model builder**

Carol, PhD student at
University of São Paulo

Johannes, PhD student
at TU Dresden

**guest talks by two
GLM experts**

With very valuable input from Paul Hanson, Hilary Dugan, Aryan Adhlukha, Matt Hipsey, Cayelan Carey, Jordan Read, Dale Robertson, Jem Stachelek, Tadhg Moore, Jorrit Mesman, Johannes Feldbauer and Annette Janssen

Welcome!

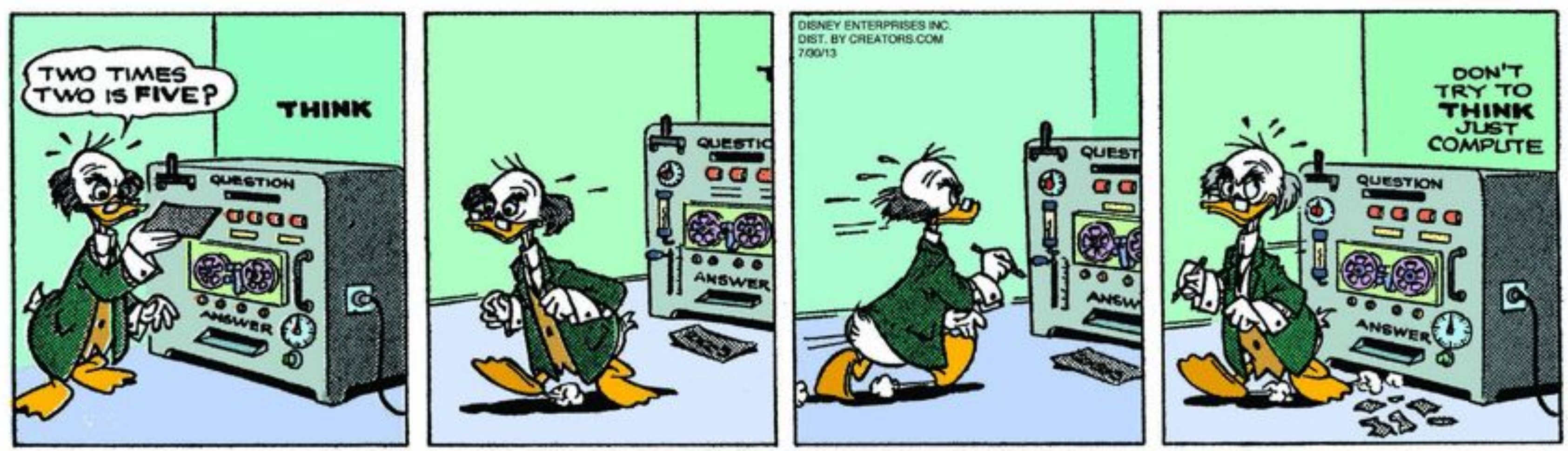
- If you want to run the simulations during the workshop, you will need to install the following software on your computer. If you just want to watch, ask questions, and drive from the back seat, that's fine, too!
- **Github**: https://github.com/robertladwig/GLM_workshop
- **Future questions?** Robert (rladwig2@wisc.edu)

(1) **Use the docker:** https://hub.docker.com/r/hydrobert/glm-workshop (requires docker)
    (a) this includes Rocker, all packages, all scripts and all data
(2) **Clone or download files** from: https://github.com/robertladwig/GLM_workshop
    (a) you'll need R (>= 4.0) and these packages: GLM3r, glmtools, rLakeAnalyzer, tidyverse

Expectations for today

- **Introduction:** to process-based modeling intended for all skill levels and background
- **Overview and hands-on coding with state-of-the-art models:** vertical 1D hydrodynamic-water quality model (**GLM**) or aquatic ecosystem and food web model (**PCLake)**

Great textbook: *Steven C. Chapra (2008) "Surface Water-Quality Modeling" Waveland Pr Inc*



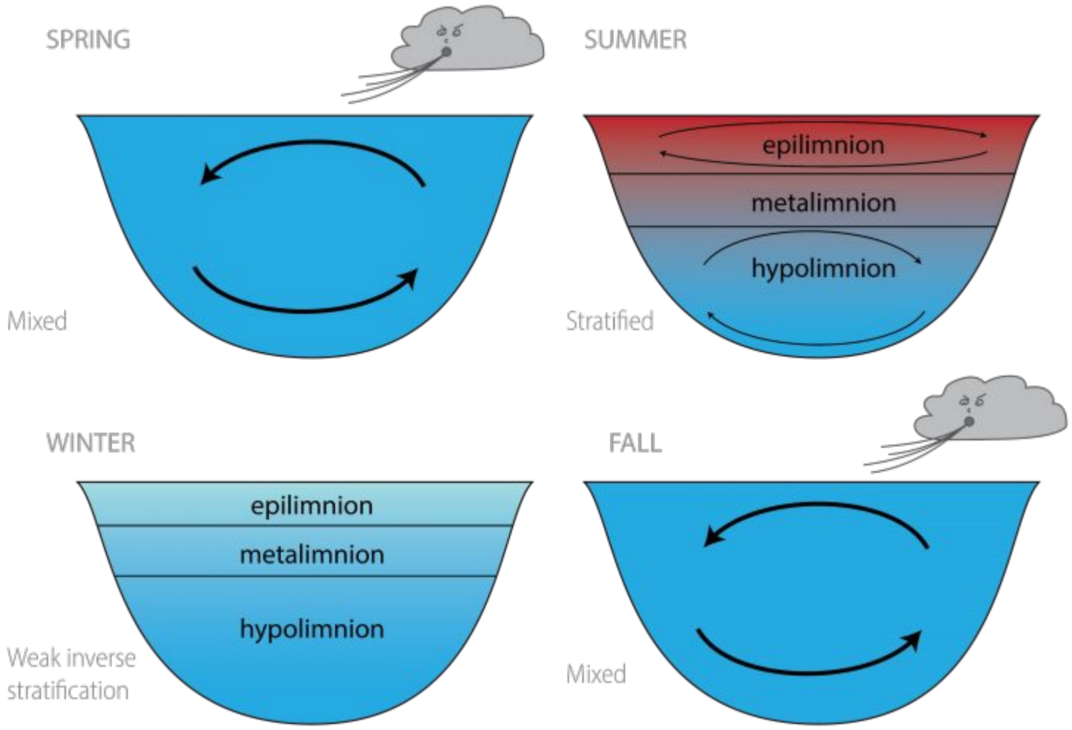
Disney's Donald Duck comics

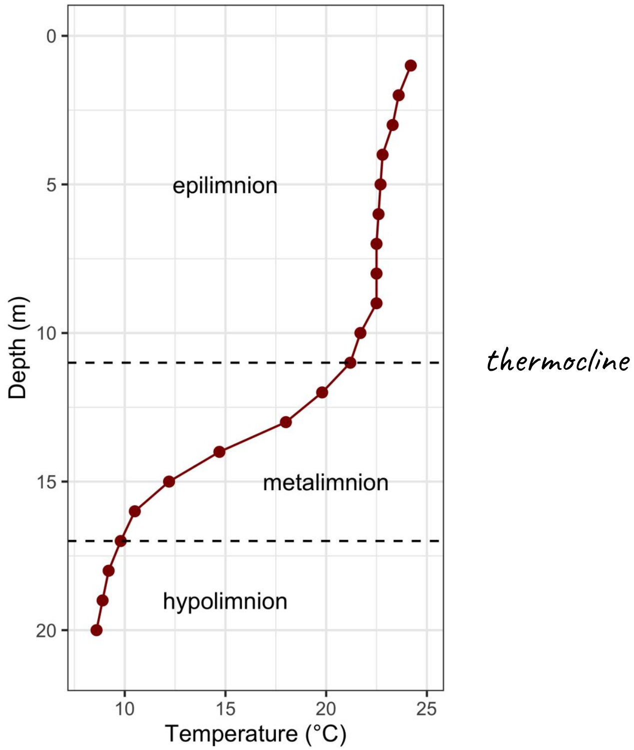
Time schedule today (all in UTC)

3:00-3:45	**Introduction to process-based aquatic ecosystem modeling**	• What is modeling? • How to approach process-based modeling? • Why should you use modeling?
4:00-5:00	**Introduction to GLM-AED2**	• Theory behind GLM and AED2 • How to set up your own model • How to work with GLM-AED2 in R
5:15-6:45	**Hands-on coding in R**	• Running the GLM-AED2 model in R • 6 different exercises • Work in sub-groups on either physics or biology

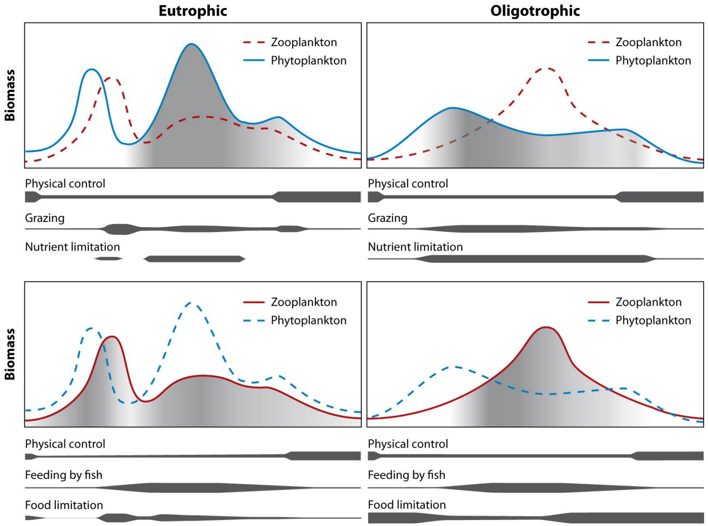
Introduction

Today we will talk about lake stratification …

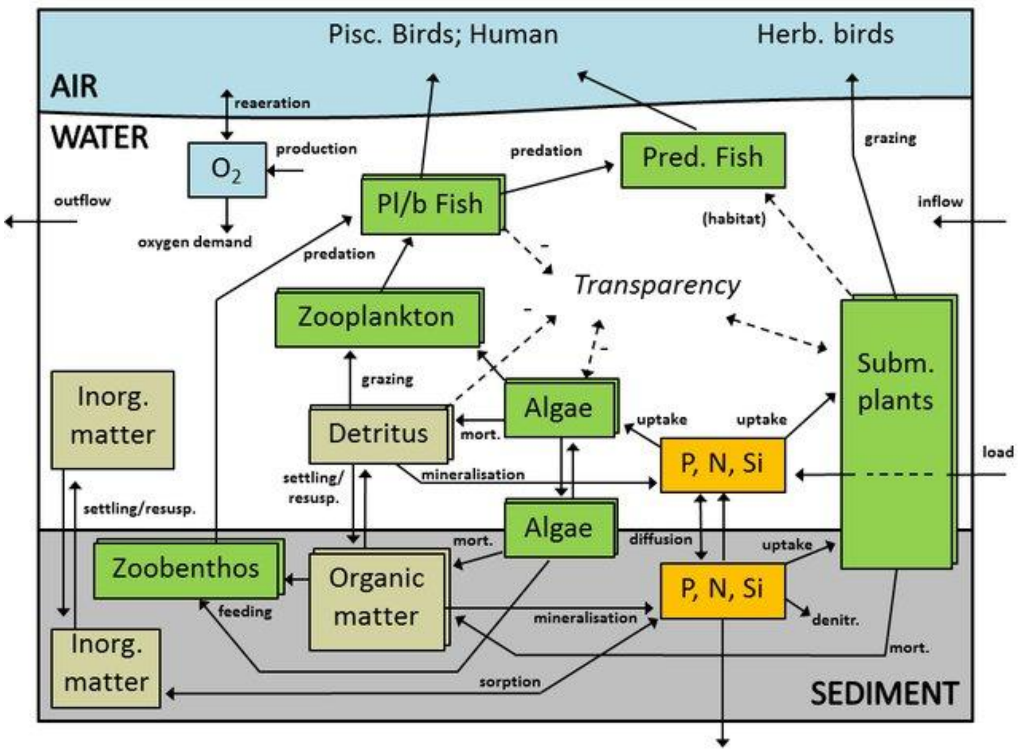




… and aquatic food webs



Sommer U, et al. 2012.
Annu. Rev. Ecol. Evol. Syst. 43:429–48



And then we have an aquatic ecosystem model (AEM)

- aquatic ecosystem modeling: *`a formal procedure by which the impact of external or internal forcing on aquatic ecosystem state(s) can be estimated`*
- two distinct classes of AEMs exist:
  - direct mathematical relation between forcing and state (statistical models)
  - formulated in terms of the processes underlying this relation (**process-based models**)

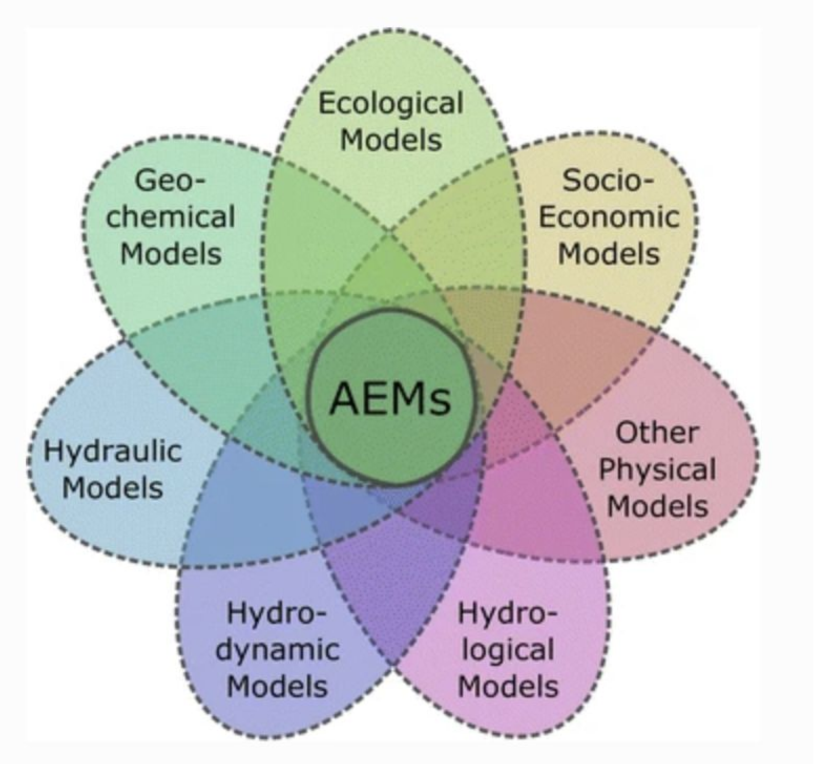
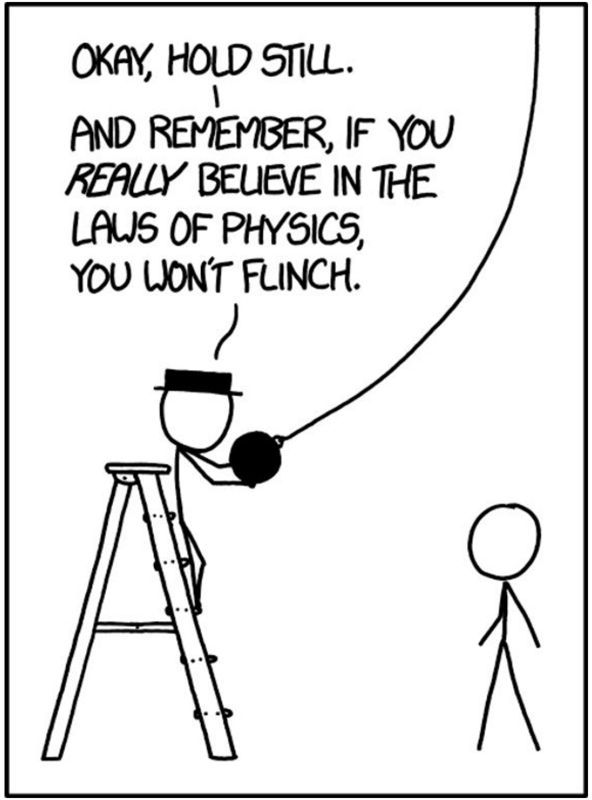


figure from Janssen et al. (2015)

First, what is modeling?

- Models are simplified reflections of reality
- Deterministic (events at next time step depend on events from previous time step)
  - and describe processes with mathematical equations
  - that are either based on empirical knowledge or physical principles
- Numerical models need time and space discretization
- As well as initial data (to start from) and boundary data (as driving data)



comic from xkcd.com

Various models exist

Which to choose?

- depends on aim
- depends on availability
- depends on your skills
- depends on the required output
- depends on key processes
- depends on your collaborators (supervisor, lab)
- depends on your budget

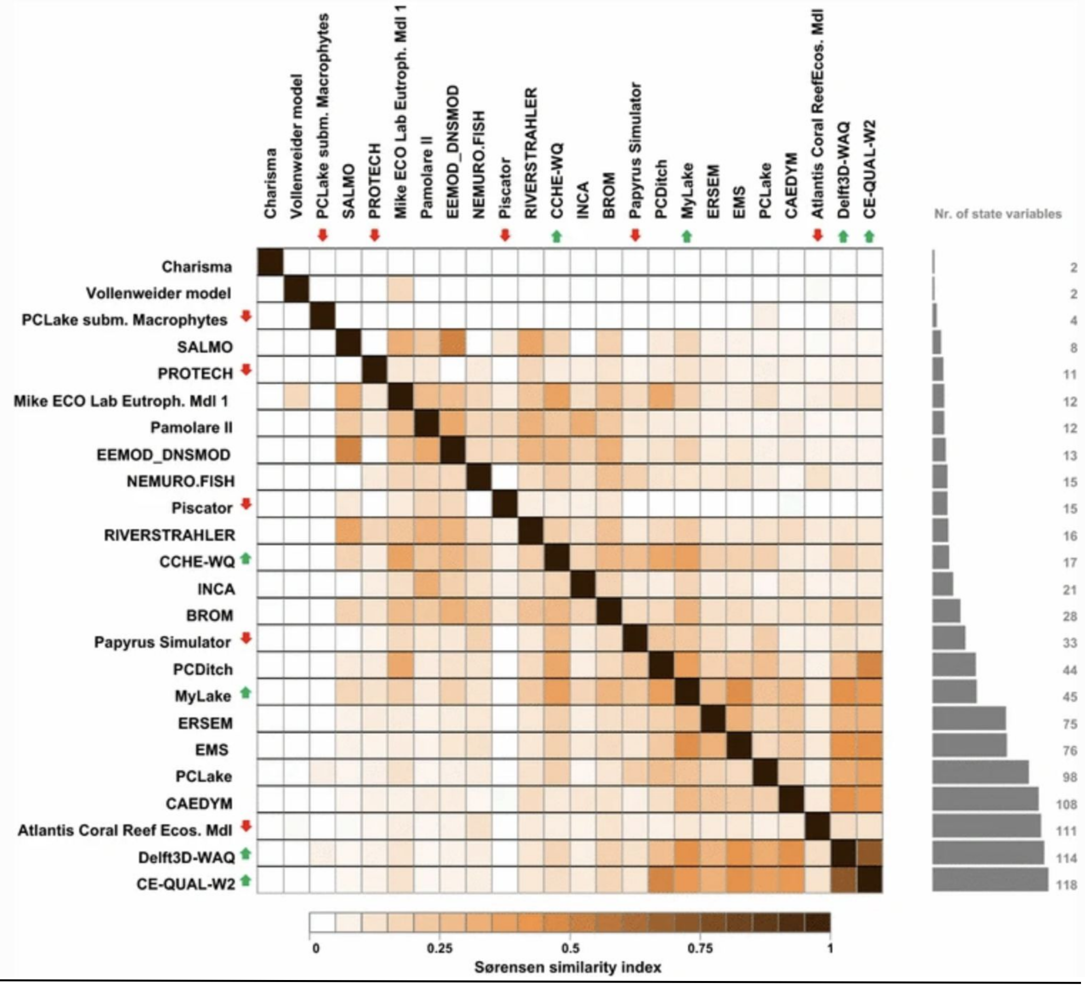
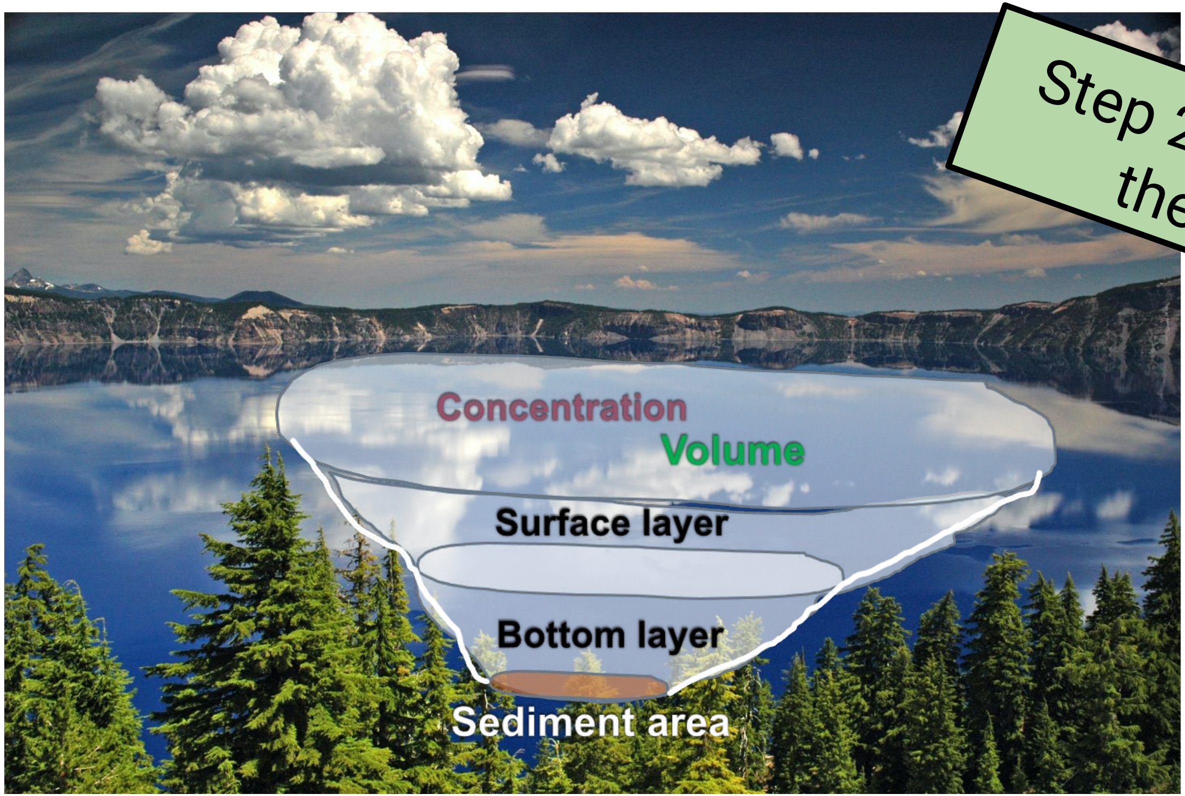


figure from Janssen et al. (2015)

Process-based modeling in a nutshell

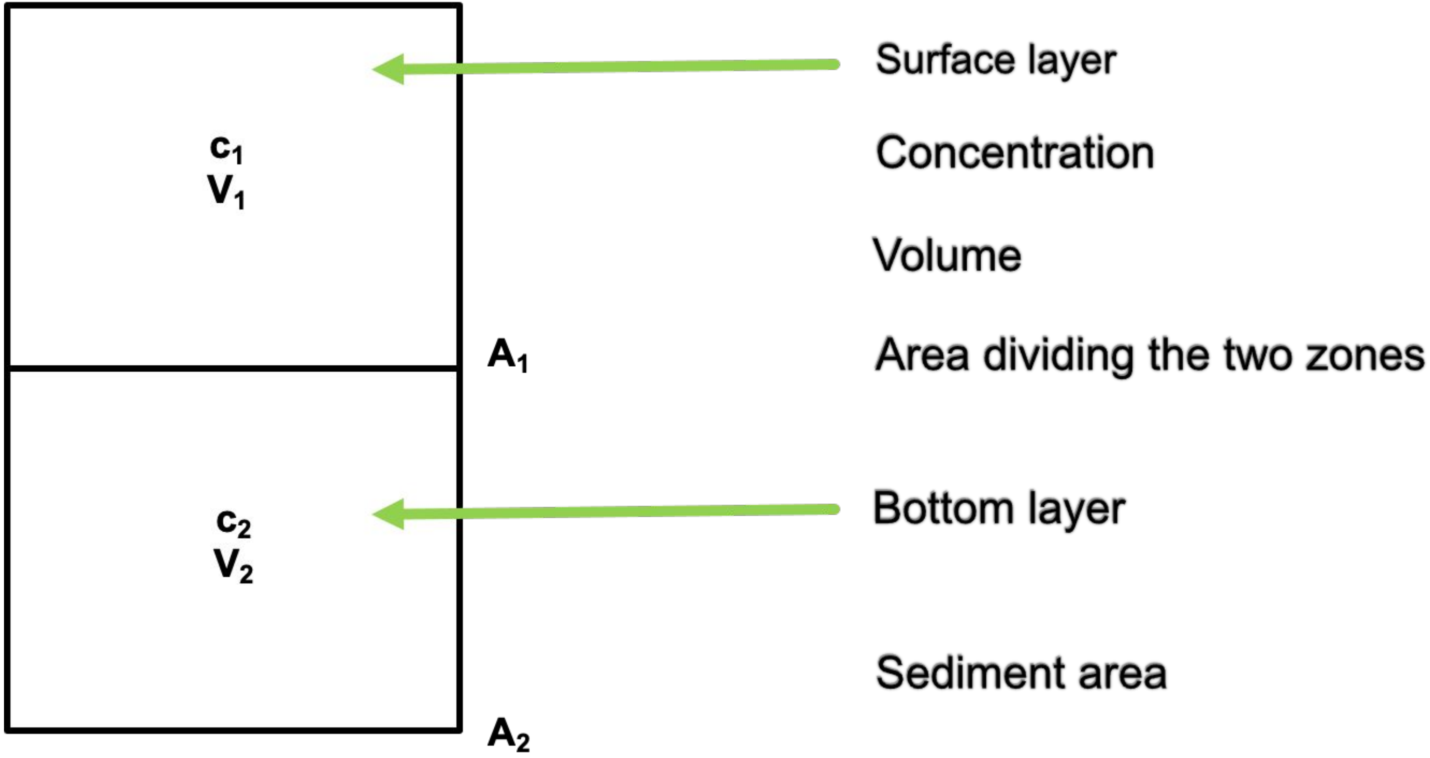
Step 1: imagine a (nice) lake

Process-based modeling in a nutshell



Step 2: abstract the lake

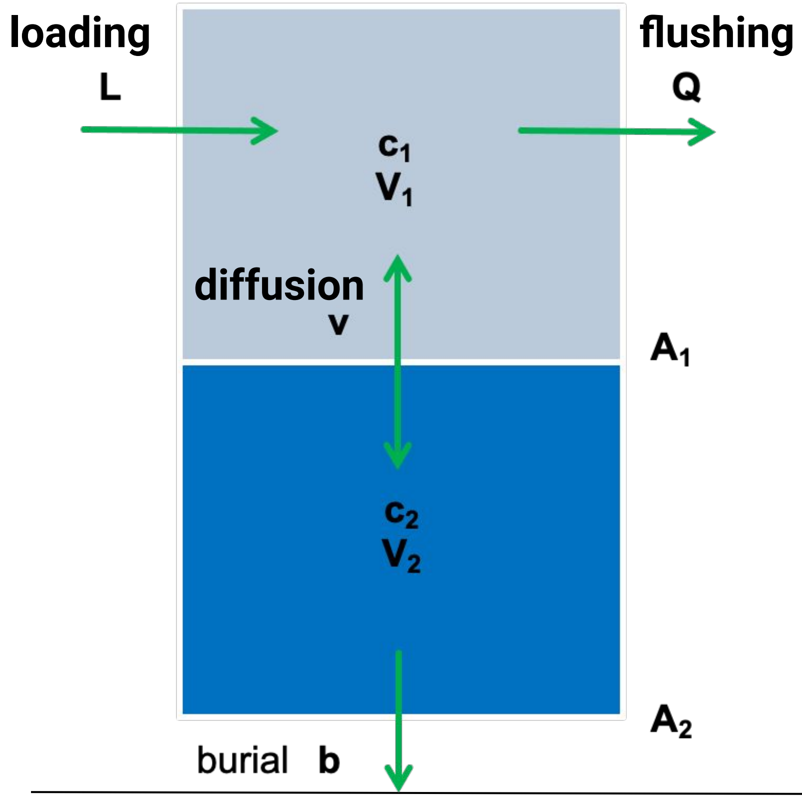
Process-based modeling in a nutshell



most are bookkeeping exercises to keep inflow = outflow (mass-balance)

Process-based modeling in a nutshell

Step 3: add math



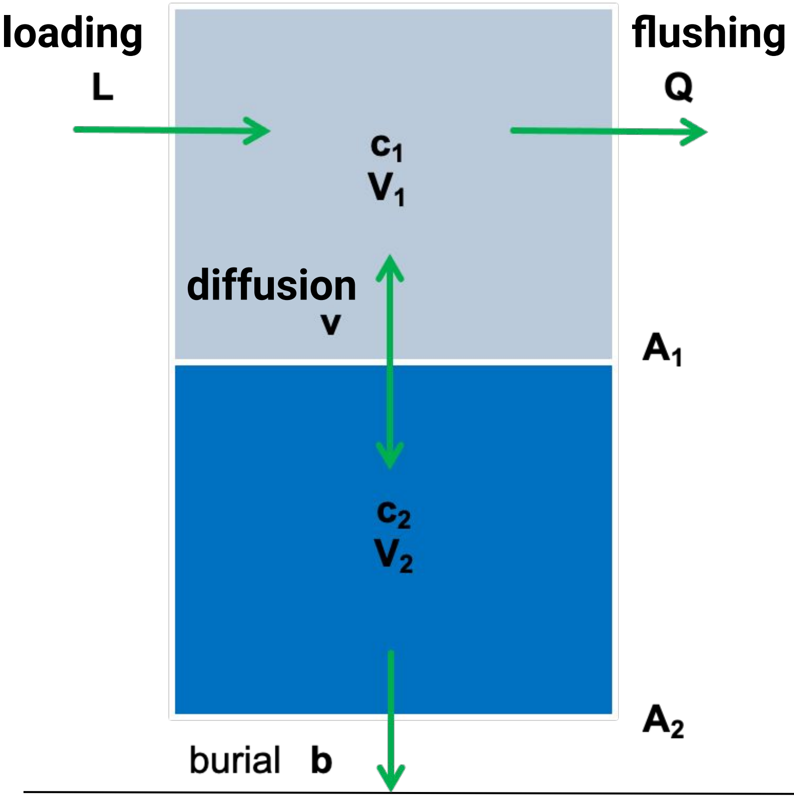
$$\frac{dc_1}{dt} = \frac{L - Qc_1 + vA_1(c_2 - c_1)}{V_1}$$

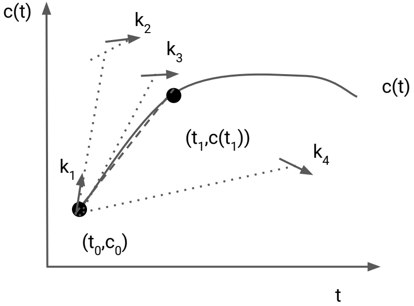
$$\frac{dc_2}{dt} = \frac{vA_1(c_1 - c_2) - bA_2c_2}{V_2}$$

most are bookkeeping exercises to keep inflow = outflow (mass-balance)

Process-based modeling in a nutshell

Step 4: solve with numerics, e.g., Runge-Kutta





$$c_{i+1} = c_i + f(c_i, t_i) * \Delta t \quad h = \Delta t$$

$$c_{i+1} = c_i + [\tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)]\Delta t$$

$$k_1 = f(t_i, c_i)$$

$$k_2 = f(t_i + \tfrac{1}{2}h, c_i + \tfrac{1}{2}hk_1)$$

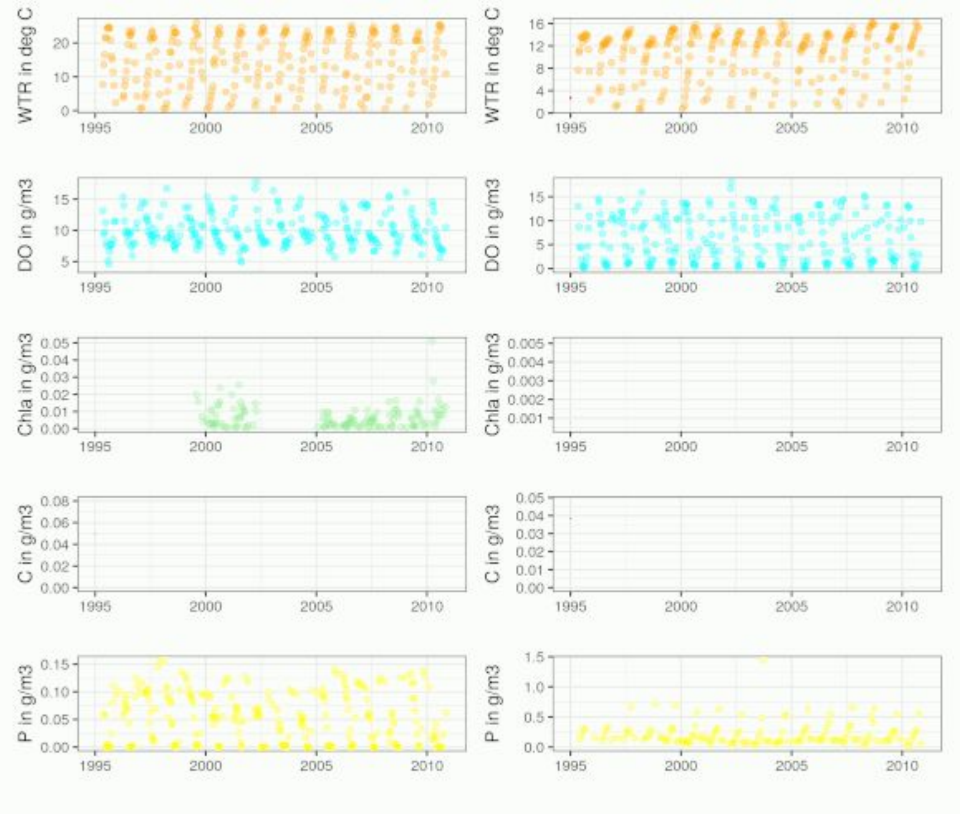
$$k_3 = f(t_i + \tfrac{1}{2}h, c_i + \tfrac{1}{2}hk_2)$$

$$k_4 = f(t_i + h, c_i + hk_3)$$

most are bookkeeping exercises to keep inflow = outflow (mass-balance)

Process-based modeling in a nutshell

- results from simple 2-layer model:
  - replicates **physics well** (thermal dynamics, water temperature)
  - **sufficient replication of biogeochemical fluxes** (oxygen, nutrients, wait - negative P?)
  - **hard time capturing biology** (phytoplankton, food webs)



results from thermod model: https://github.com/robertladwig/thermod

What are the laws?

- **Conservation of mass (continuity)**
  - source = sink (+ storage)
  - Mass cannot be created or destroyed

- **Conservation of momentum**
  - Velocity based on balances of forces (gravity, pressure, friction, earth-rotation)

State of the environment

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = q_0$$

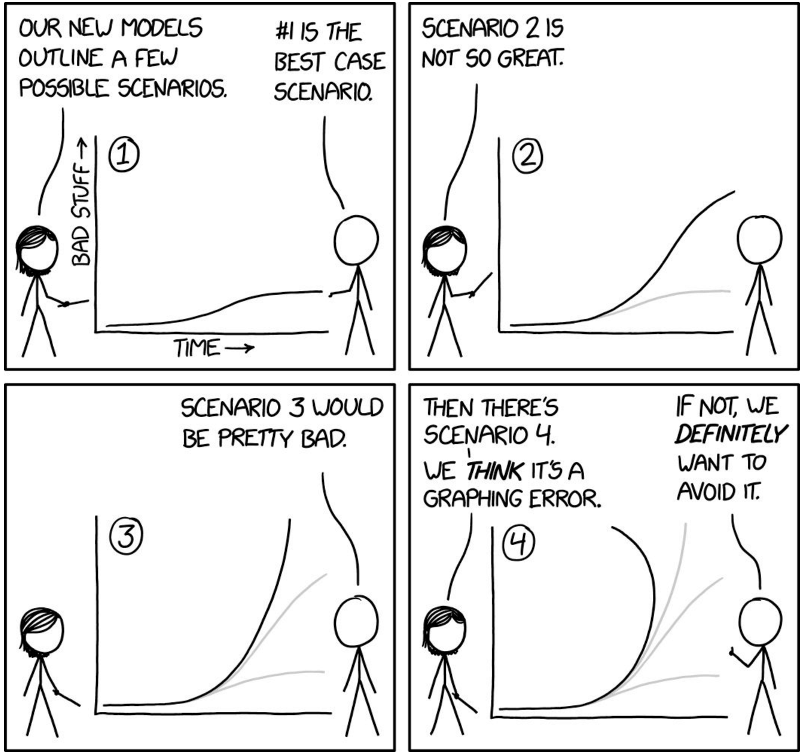
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\nabla\mathbf{v} = -\frac{1}{p}\nabla p + g + \nu\Delta\mathbf{v}$$

State of the system

Process-based modeling in a nutshell

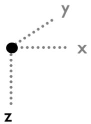
Why should you use a model?

- Explore ideas regarding ecological systems that <u>may not</u> be possible/feasible to field-test for
  - logistical, political, financial and/or physical reasons
- Formulating a model helps to better understand the system and can identify data needs → repetitive experiments
- test environmental constraints/thresholds
- “Your model is your hypothesis.” (Kate)



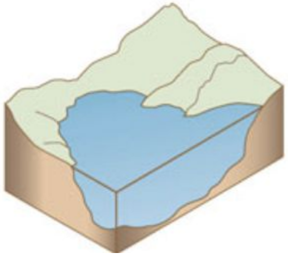
Evans 2010; comic from xkcd.com (last comic in this presentation, I swear)

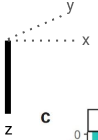
Model dimensions



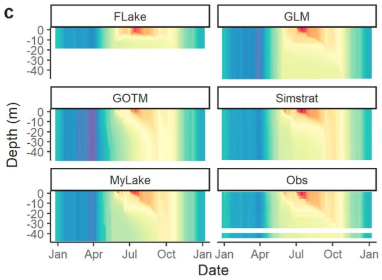
zero-dimensional

0D: Box model

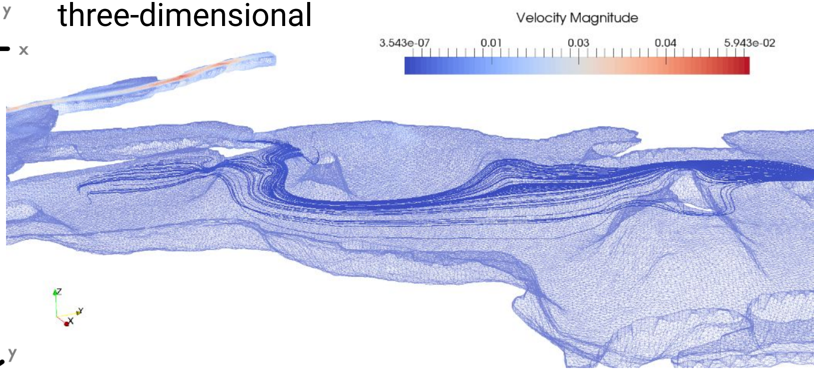


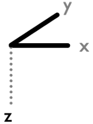


vertical 1D

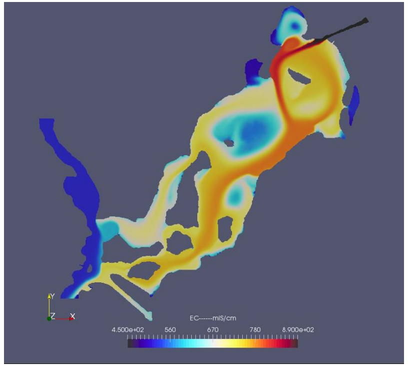


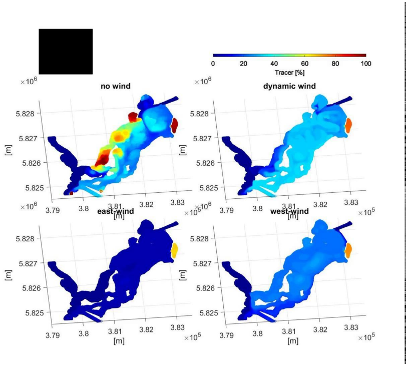
three-dimensional



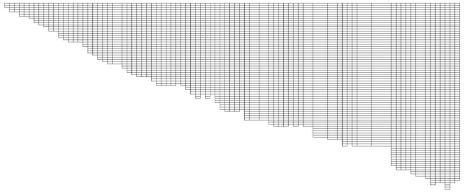


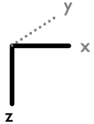
depth-averaged 2D





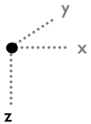
longitudinal-vertical 2D





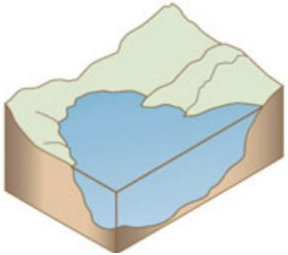
0D model: Trolle et al. 2012; 1D model: Moore et al. 2021; longitudinal-vertical 2D model: Mi et al. 2020

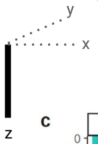
Model dimensions



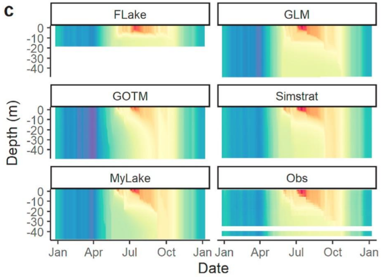
zero-dimensional

0D: Box model

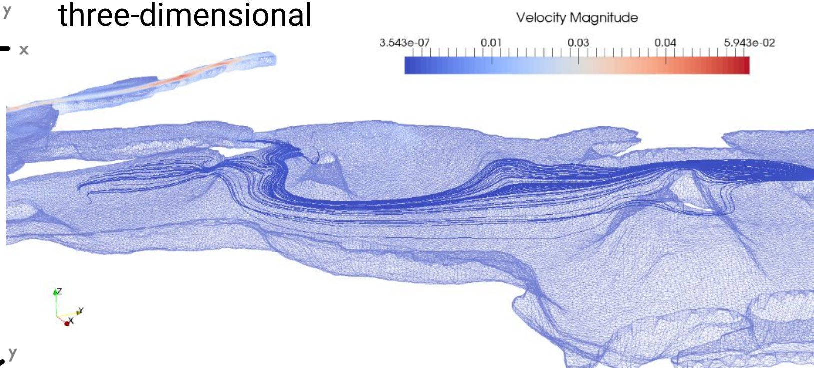


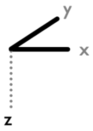


vertical 1D

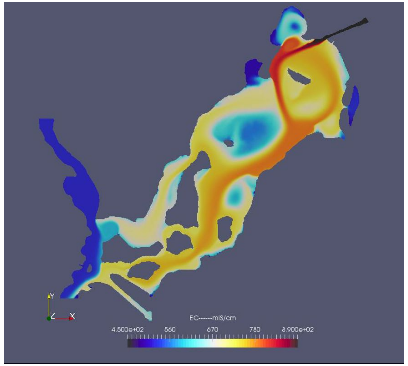


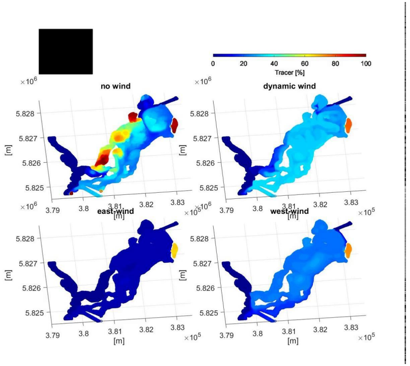
three-dimensional



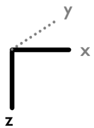


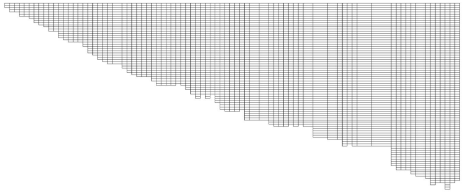
depth-averaged 2D





longitudinal-vertical 2D



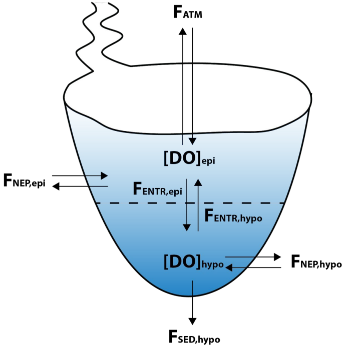


0D model: Trolle et al. 2012; 1D model: Moore et al. 2021; longitudinal-vertical 2D model: Mi et al. 2020

Learn from the expert: *Modeling of carbon dynamics in lake systems*

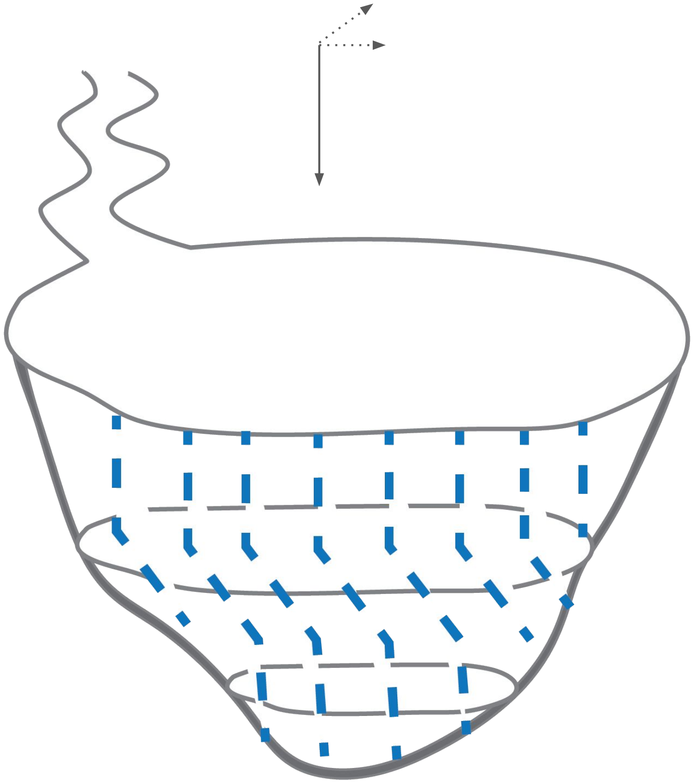
Austin Delany: Master of Science thesis at UW-Madison in the Paul Hanson team

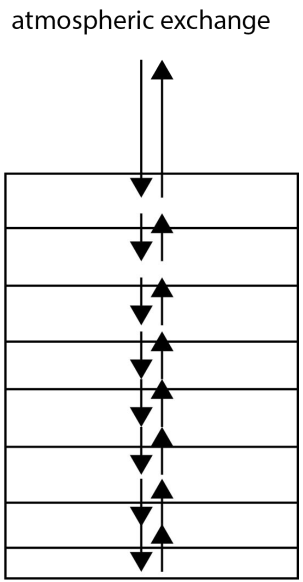
- coded his own aquatic ecosystem model in R with feedbacks for organic carbon, light, oxygen, phosphorus and temperature dynamics



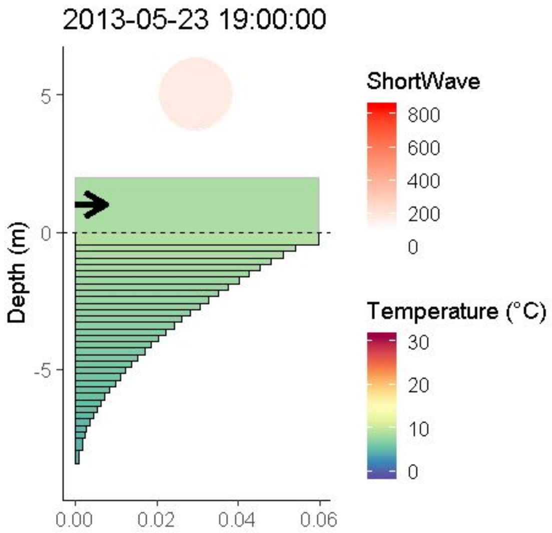
The General Lake Model (GLM) a: introduction

Process-based lake modeling





- **Vertical 1D model**:
  - Horizontal homogeneity
  - No Coriolis force
- Layering over vertical axis
- Every layer = volume of lake
- **Focus on heat transport**



layer animation by Tadhg Moore

Process-based lake modeling

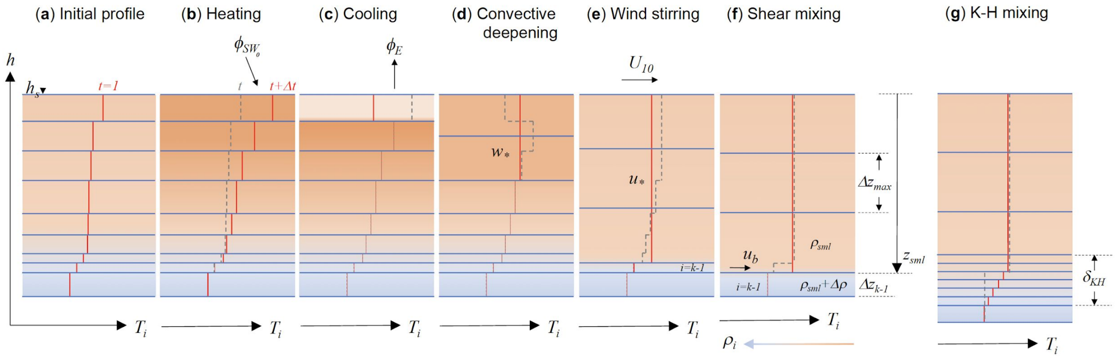
- reactive-diffusive transport equation for water temperature
  - turbulence-closure scheme to solve for momentum terms and diffusivities (e.g., k-ε in Simstrat)
- **GLM (General Lake Model)**: energy-balance approach: potential ag. available kinetic energy → heat transport

$$\frac{\partial T}{\partial t} = \frac{1}{A}\frac{\partial}{\partial z}\left(A(v_t' + v')\frac{\partial T}{\partial z}\right) + \frac{1}{\rho_0 c_p}\frac{\partial H_{sol}}{\partial z} + \frac{dA}{dz}\frac{H_{geo}}{A\rho_0 c_p}$$

diffusive transport | atmospheric heating | sediment heating

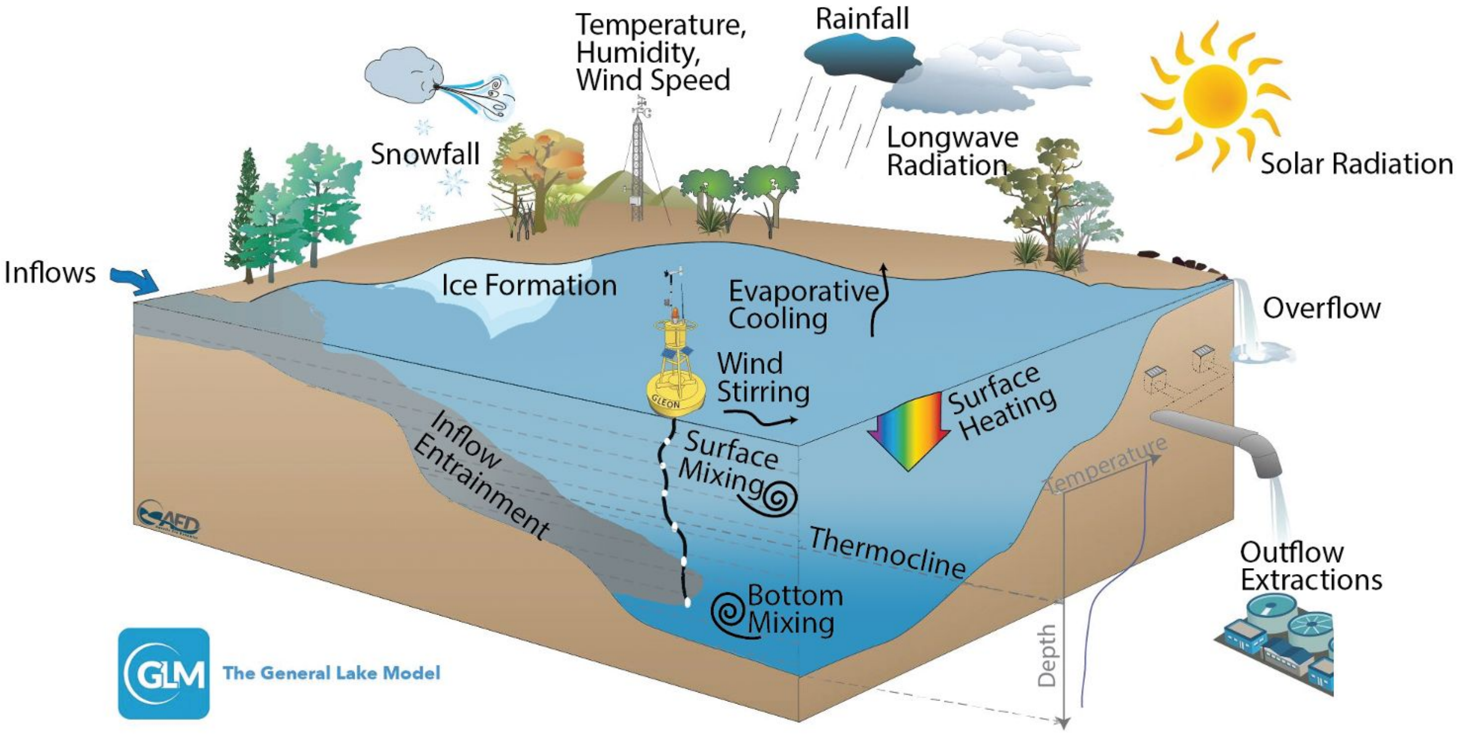
$$E_{TKE} = \underbrace{0.5C_K(w_*^3)\Delta t}_{\text{convection}} + \underbrace{0.5C_K(C_W w_*^3)\Delta t}_{\text{wind stirring}} + \underbrace{0.5C_S[U_b^2 + \frac{U_b^2}{6}\frac{d\xi}{dz_{SML}} + \frac{u_b\xi}{3}\frac{du_b}{dz_{SML}}]}_{\text{shear production, K-H production}}\Delta z_{k-1} \quad (5)$$

$$E_{PE} = \underbrace{[0.5C_T(w_*^3 + C_W u_*^3)^{2/3}}_{\text{acceleration}} + \underbrace{\frac{\Delta\rho}{\rho_0} g z_{SML}}_{\text{lifting}} + \underbrace{\frac{g\xi^2}{24\rho_0}\frac{d(\Delta\rho)}{dz_{SML}} + \frac{g\xi\Delta\rho}{12\rho_0}\frac{d\xi}{dz_{SML}}]}_{\text{K-H consumption}}\Delta z_{k-1} \quad (6)$$



Simstrat: Goudsmit et al. 2002, MyLake: Saloranta and Andersen 2007, GLM: Hipsey et al. 2019

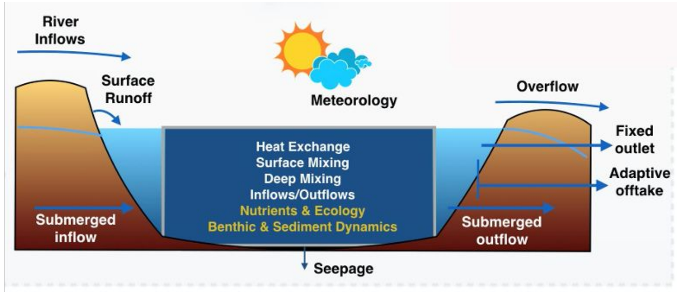
General Lake Model (GLM)



Hipsey et al. 2019

General Lake Model (GLM)

- GLM started as a GLEON project
- Developed by Matt Hipsey, Louise Bruce and Casper Boon at UWA
- Designed to operate with the Aquatic EcoDynamics Model Libraries (AED2) → water quality model
- Written in C and Fortran
- Freely available as open-source program: https://github.com/AquaticEcoDynamics/GLM



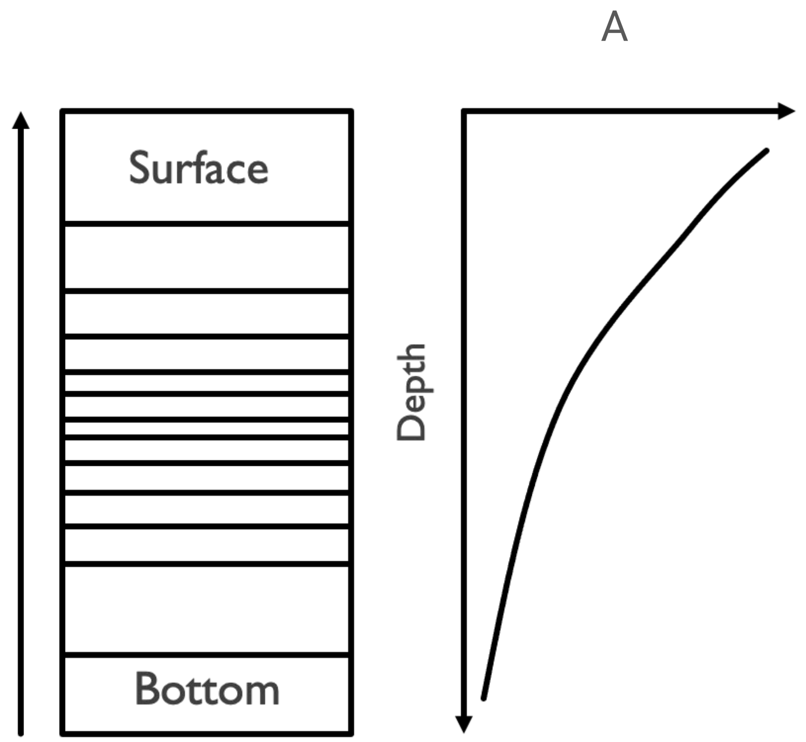
The General Lake Model (GLM) b: hydrodynamics

Grid

- Each vertical layer (= control volume) adapts its thickness due to flows, mixing and mass fluxes

  → flexible Lagrangian structure

- Each layer has ‘unique’ density
- When there’s enough energy to overcome density gradient → layers merge
- Layer’s volume changes depending on hypsography



Hipsey et al. 2019

Grid

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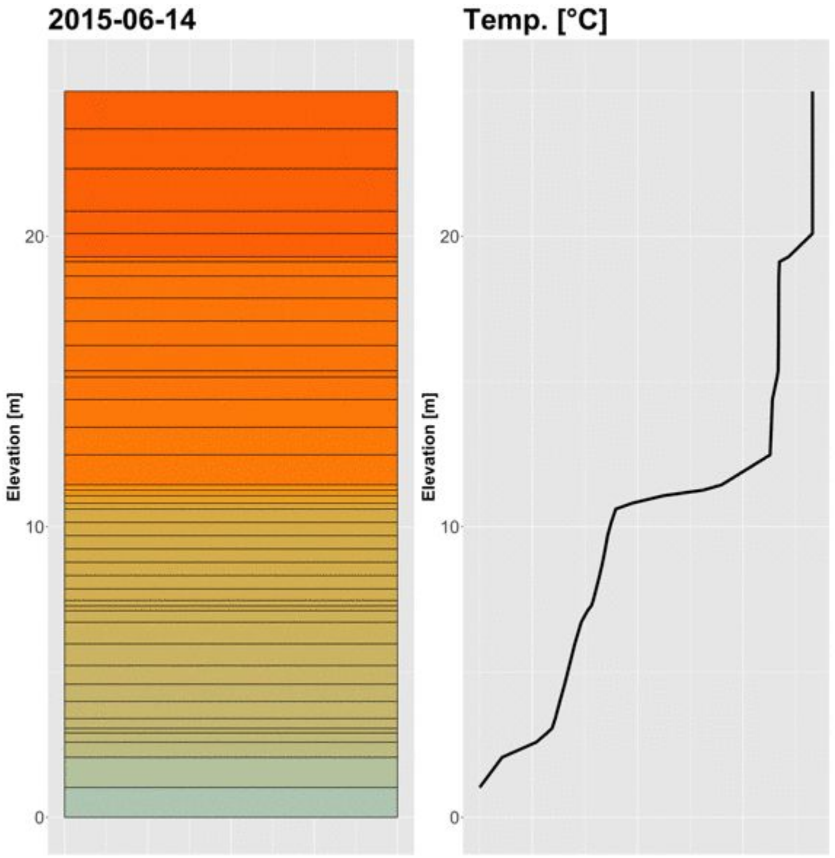
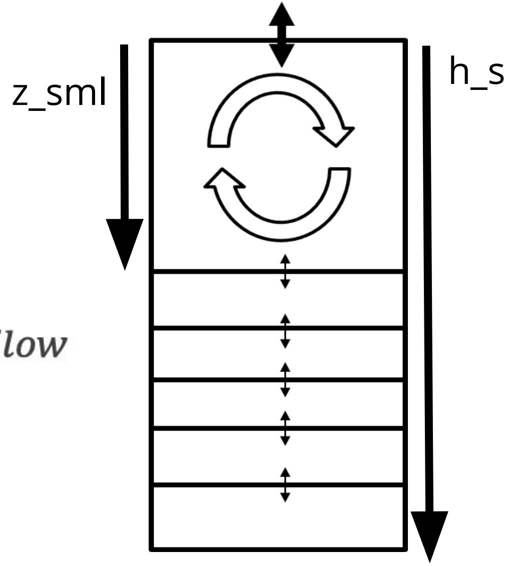


Hipsey et al. 2019

Water balance



- Net water flux over total lake (solved by integration over time):

$$\frac{dV_s}{dt} = A_s \frac{dh_s}{dt} + \Sigma_I^N Q_{inf,I} - \Sigma_I^N Q_{out,I} - Q_{seepage} - Q_{overflow}$$

Surface layer height

- Code solves first for surface flux changes, then for all other fluxes

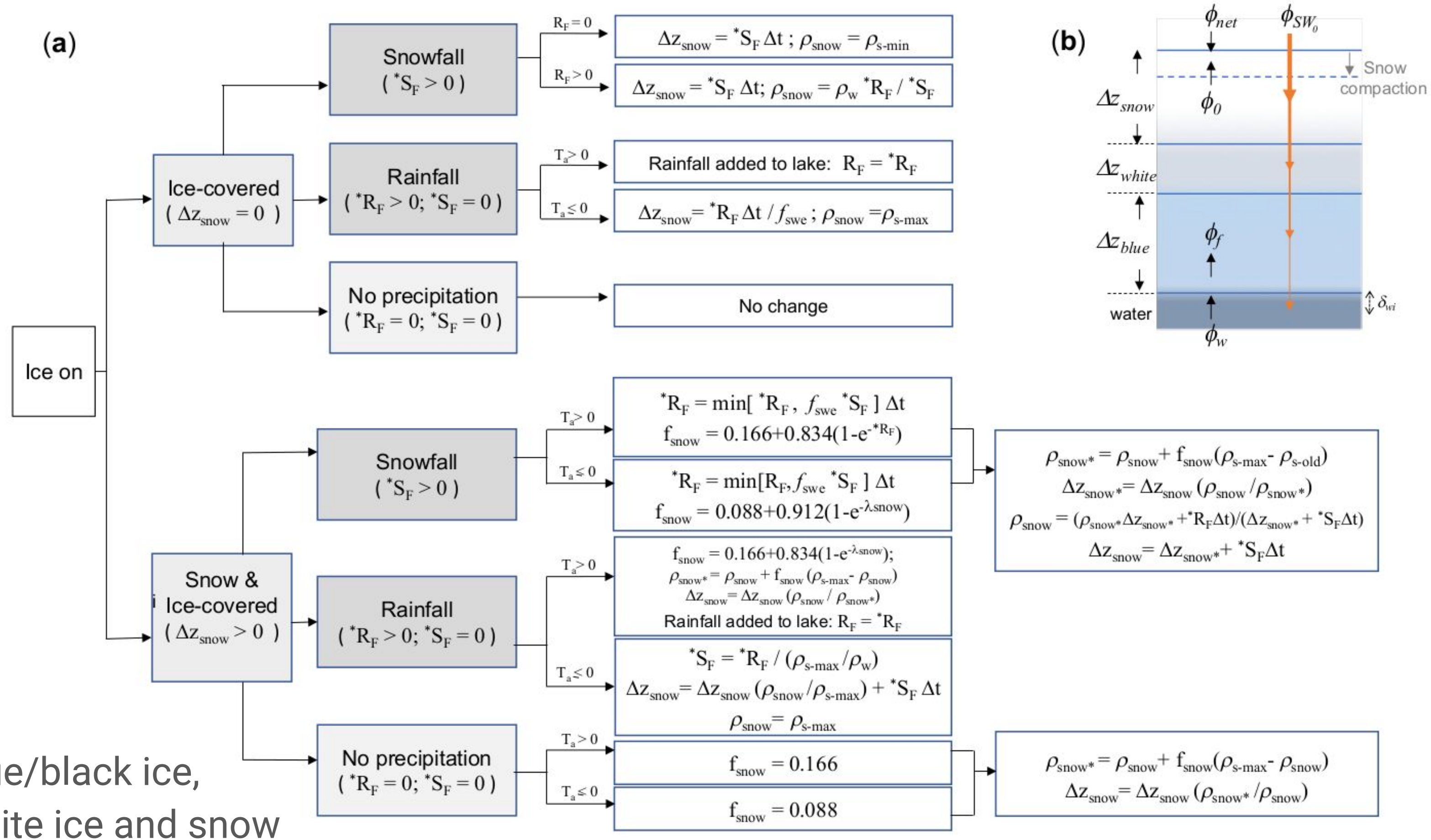
Mass balance of surface layer = precipitation + snowfall + run-off – evaporation - ice

$$\frac{dh_s}{dt} = P + S + \frac{Q_R}{A_S} - E - \frac{d\Delta z_{ice}}{dt}$$

- Mixing only affects thickness of surface layer (z_sml) not its height

Hipsey et al. 2019

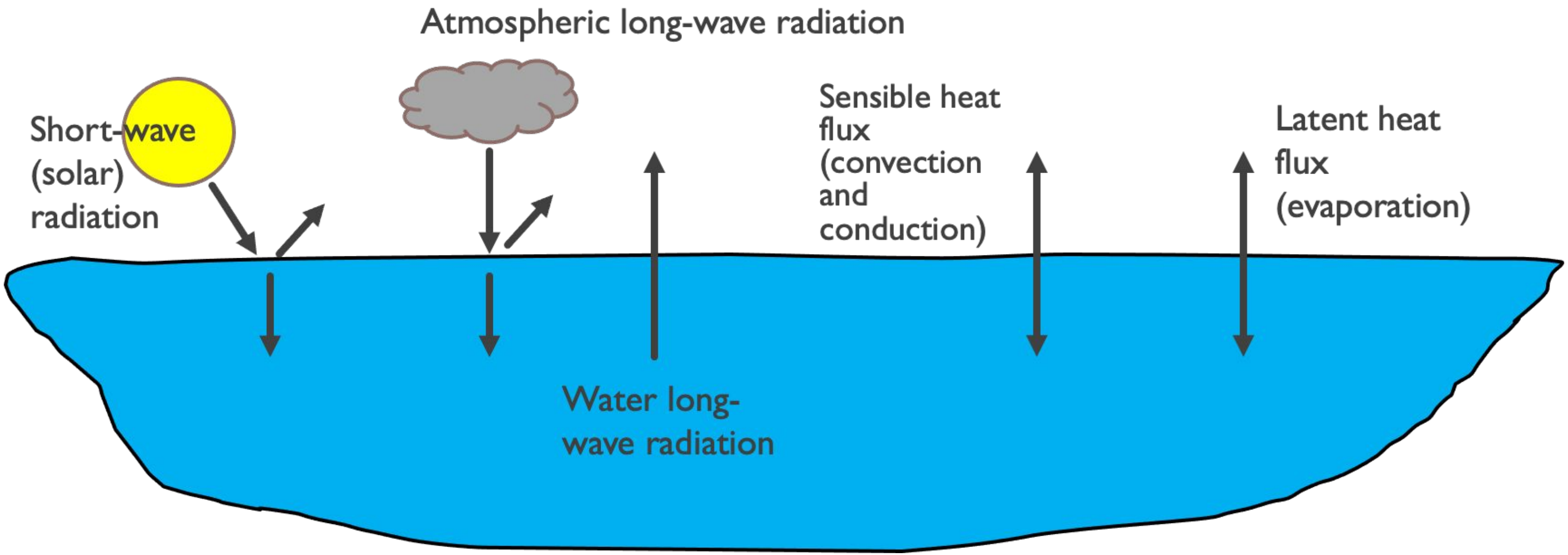
Snow and ice dynamics



blue/black ice,
white ice and snow

Surface energy balance

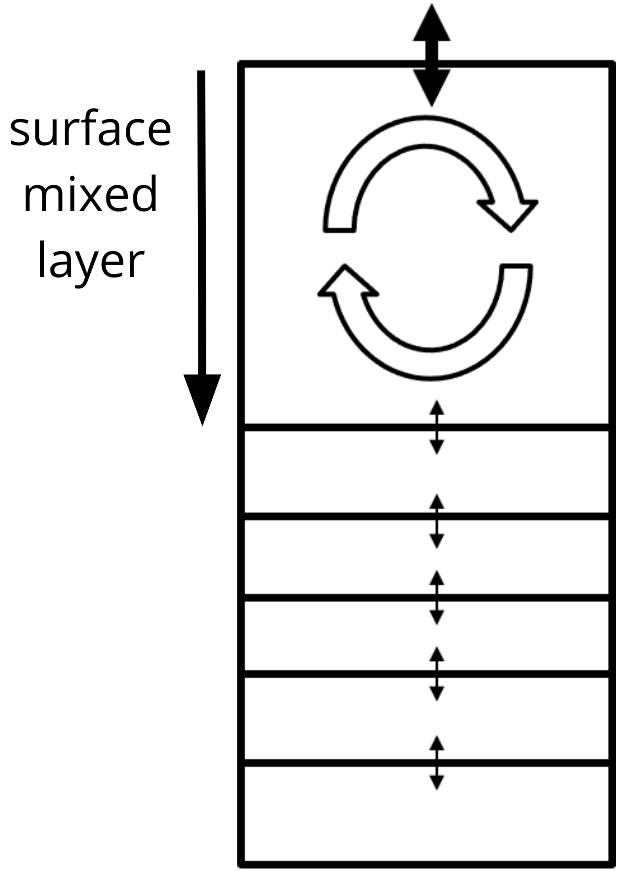
$$\rho C_p z_s \frac{dT_s}{dt} = J_{SW} + J_{LW,in} - J_{LW,out} - J_E + J_H$$



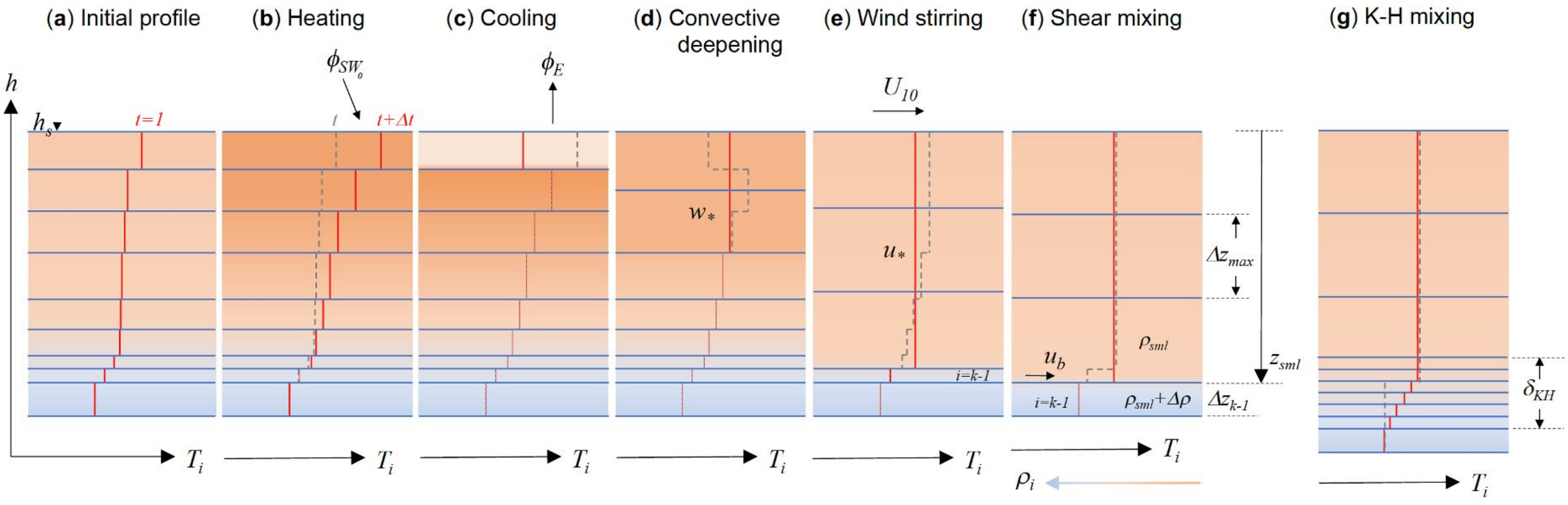
Hipsey et al. 2019

Mixing I

- Surface layer: energy balance approach
  - Energy balance determines thickness of surface mixed layer
  - Below surface mixed layer, turbulent diffusion approach is used
- Here, mixing depends on <u>difference between potential energy and available kinetic energy</u>
- Kinetic energy = convective overturn, wind stirring and shear production/Kelvin-Helmholtz billowings

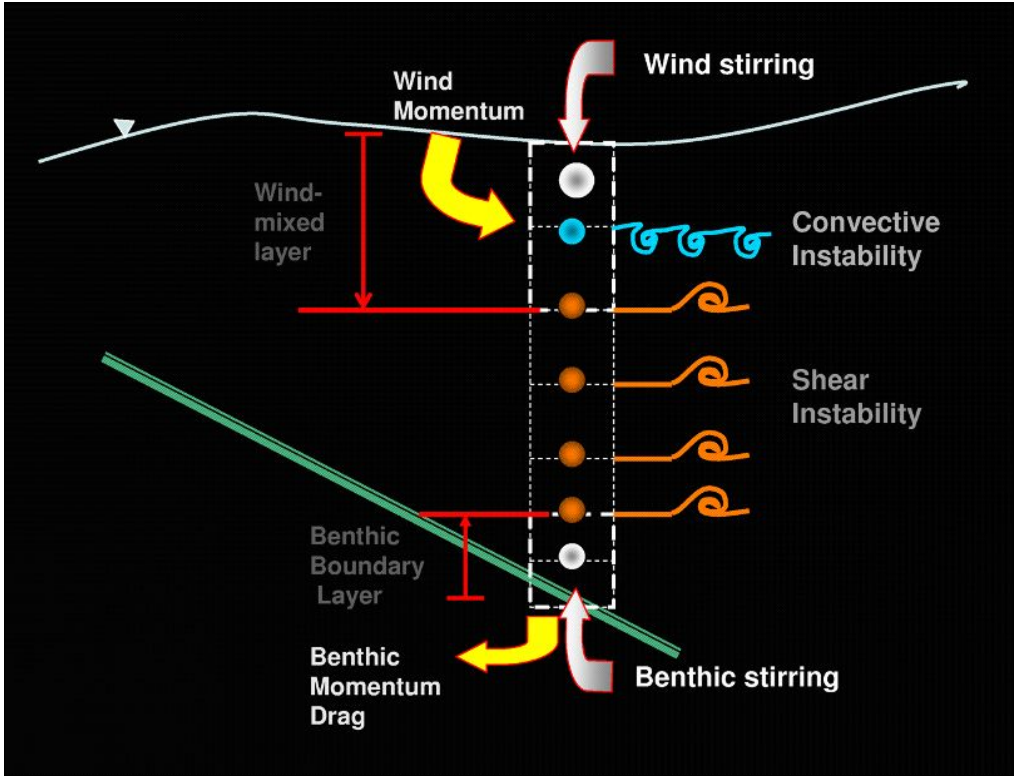


Mixing II



Hipsey et al. 2019

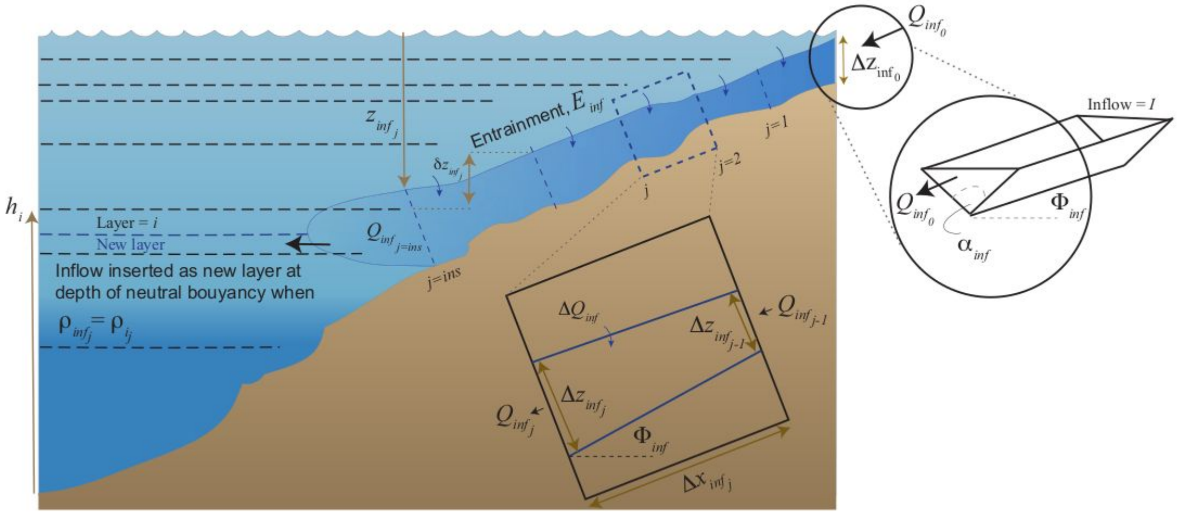
Mixing III



Kelvin-Helmholtz instabilities

Inflow and outflow dynamics

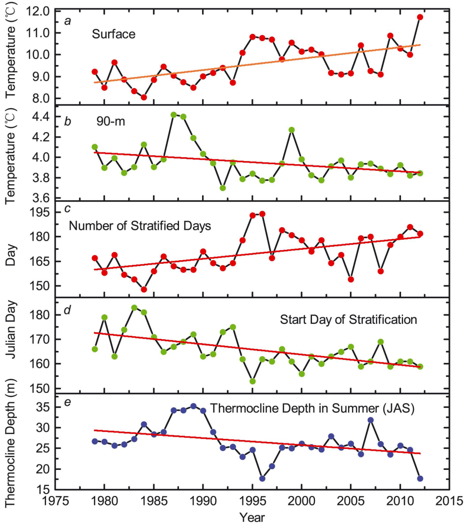
- inflows can be riparian run-off, river inflows (either buoyant or plunge) or submerged inflow (groundwater)
- outflows can be depth-specific withdrawal (reservoirs), adaptive offtake (reservoirs), groundwater seepage or river outflow; everything else = overflow



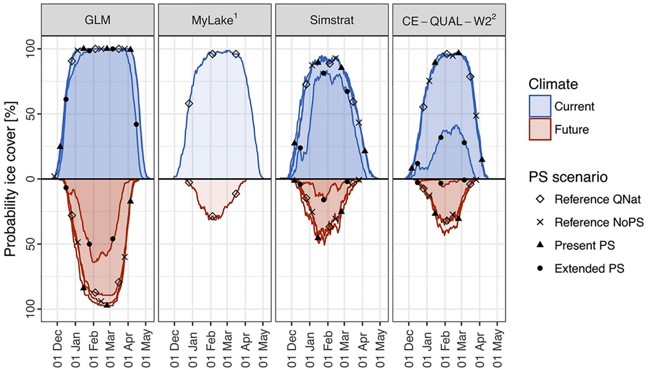
Hipsey et al. 2019

Example applications

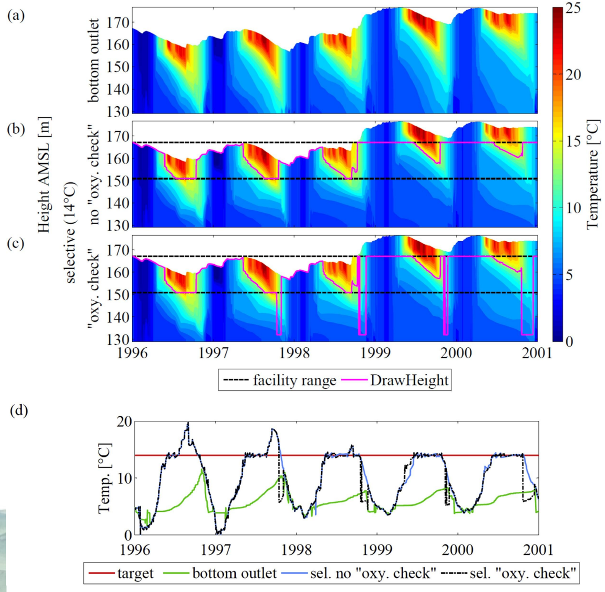
Climate change effects on lakes[1]

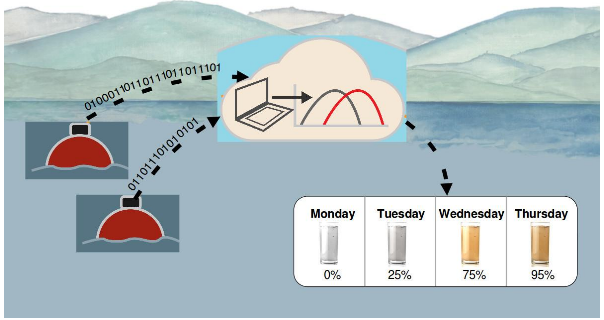


Future ice cover shifts[2]



Optimal withdrawal depth in reservoirs[4]





Smart ecological forecasting (FLARE)[3]

Learn from the expert: *Climate change impact on Brazilian reservoirs*

C.C. Barbosa, M.C. Caliijuri, A.C. Albe dos Santos, R. Ladwig, L.F.A de Oliveira, and A.C.Sarmento: Future projections of water level and thermal regime changes of a multipurpose subtropical reservoir (Sao Paulo, Brazil), Science of the Total Environment **770**, 144741 (2021)

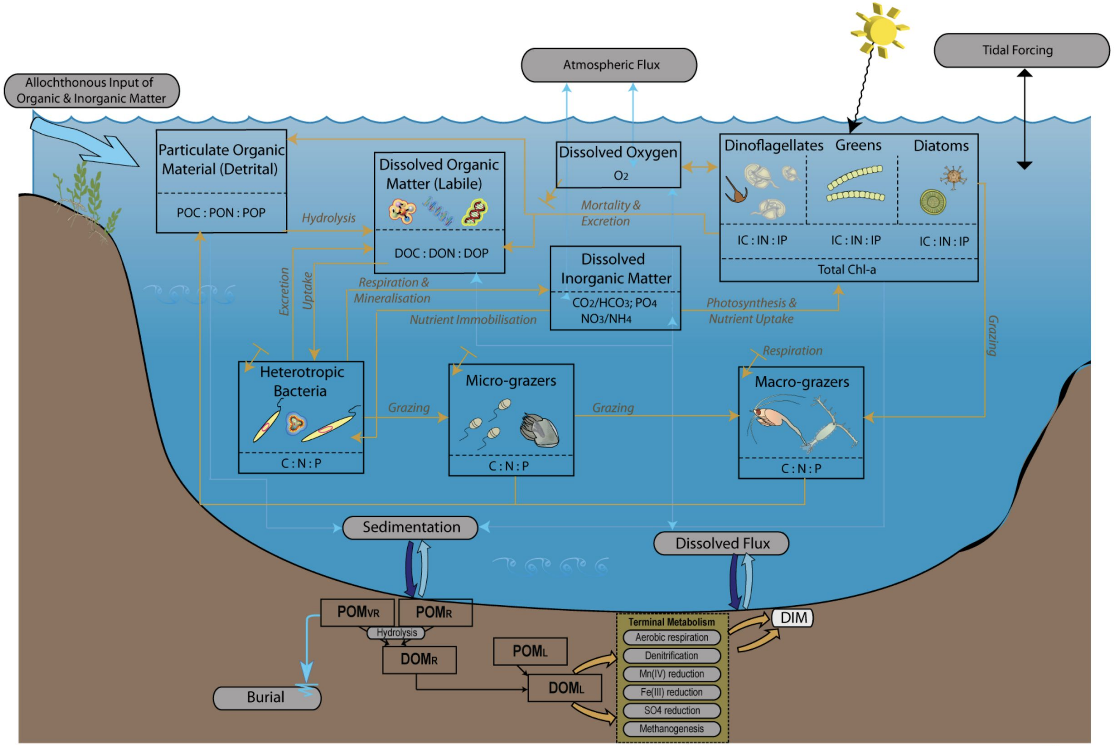
- GLM to project water level changes in reservoir → threat of dead storage

GLM

The General Lake Model (GLM) c: water quality

AED2: water quality model

- Coupled to GLM
- Conceptualize your individual ecosystem:
  - Oxygen, nutrients, phytoplankton
  - Sediment biogeochemistry
  - Benthic communities

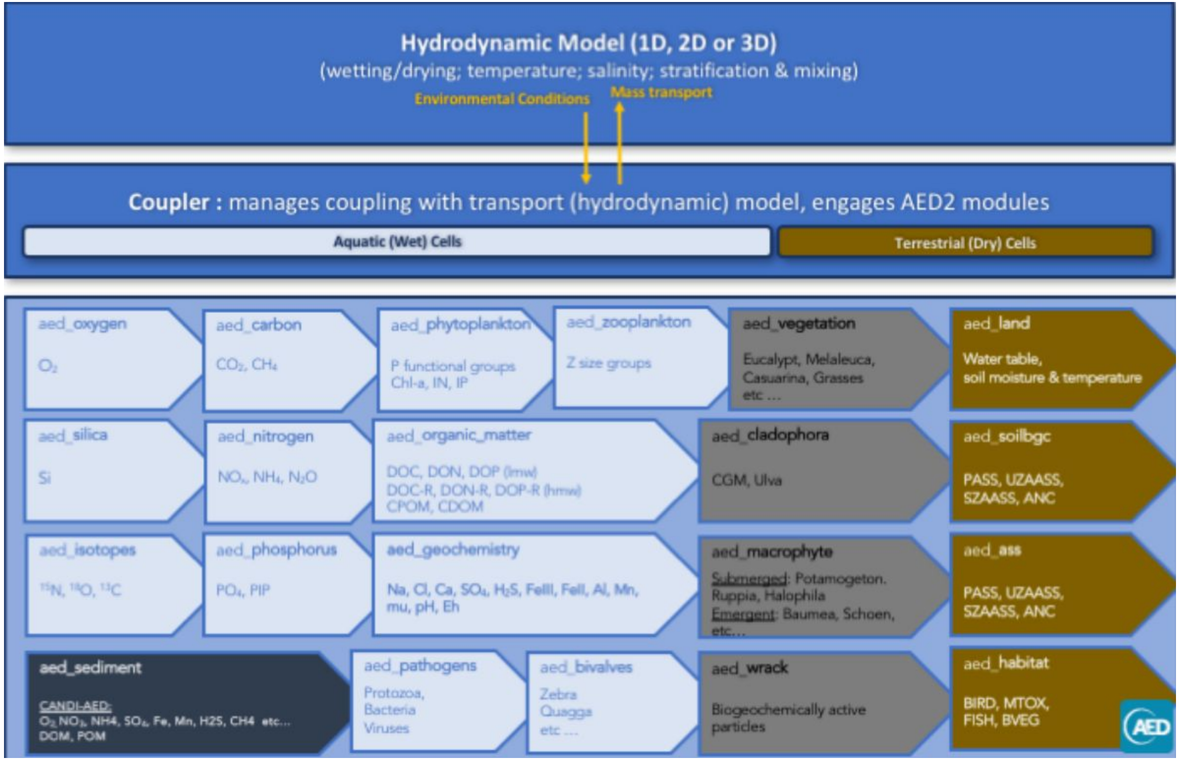


Carbon & Nutrient Flux Pathways

AED2 manual: Hipsey et al. 2013

AED2: modularised structure

- Interacts with GLM (two-way coupling)
- Array of modules are available
- Hierarchy of dependencies between modules, e.g., nitrogen reactions can depend on availability of oxygen



AED2 homepage: https://aed.see.uwa.edu.au/research/models/aed/index.html

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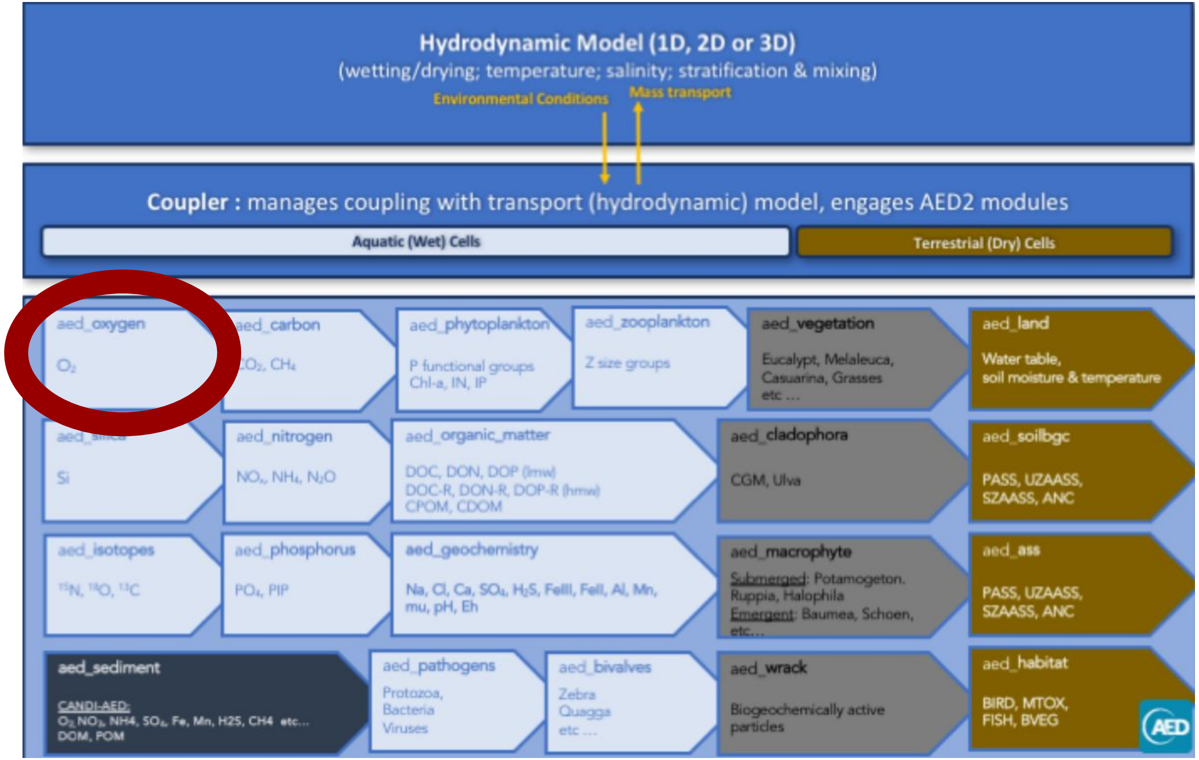
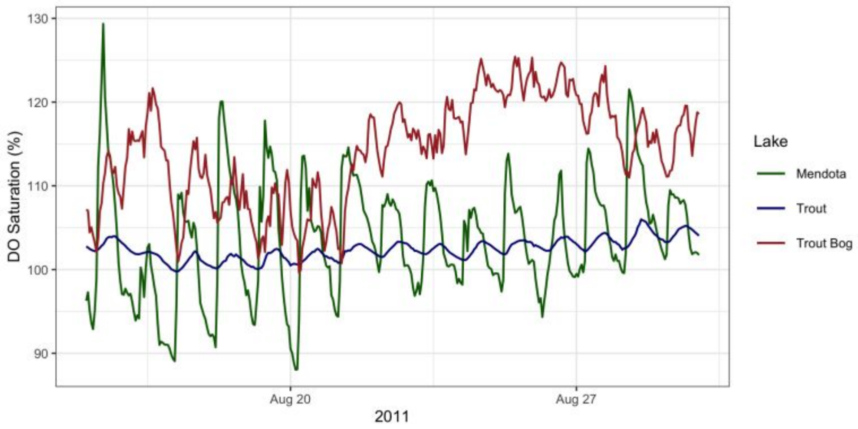


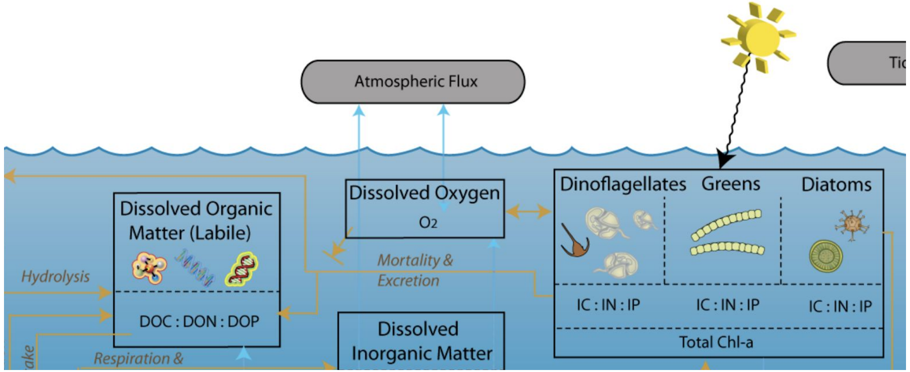
AED2: dissolved oxygen

atmospheric exchange   sediment oxygen demand

$$F_{[DO]}^{total} = k_{O_2}([DO]_{air} - [DO]_{water}) + S_{SOD} f_{SOD}^{T}(T) f_{SOD}^{DO}(DO) +$$
$$F_{mineralisation} +$$
$$F_{nitrification} +$$
$$F_{photosynthesis} +$$
$$F_{respiration}$$

- Fast moving pool (minutes to days)
- Solved over vertical axis
- Plus advection and diffusion
- Photosynthesis/respiration = phytoplankton, zooplankton, seagrass, bivalves





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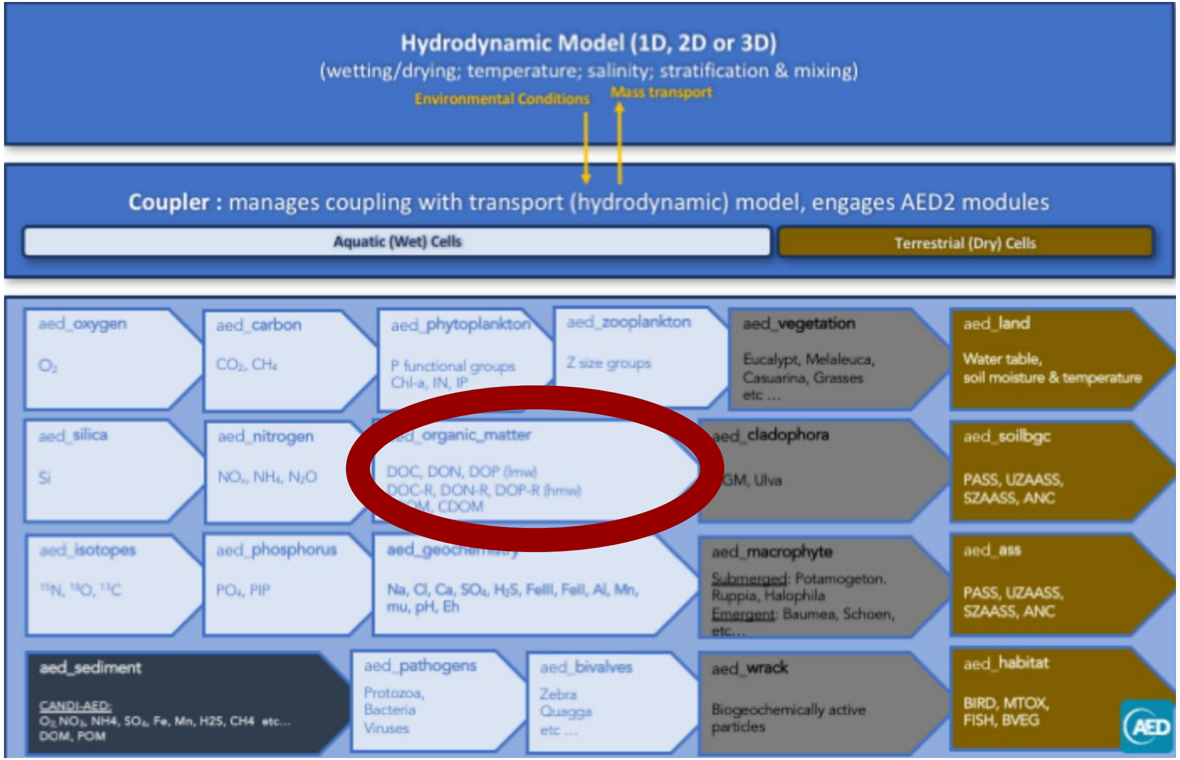
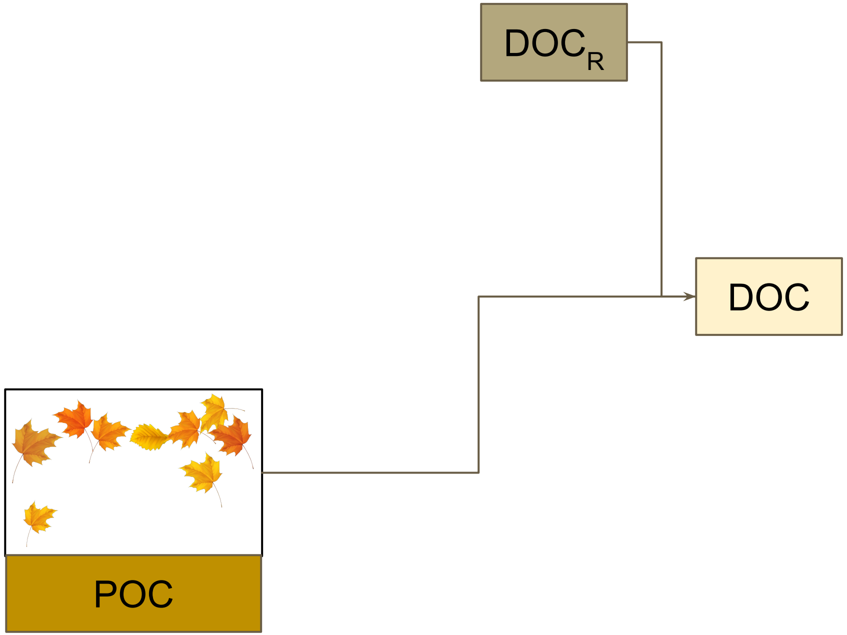


AED2 homepage: https://aed.see.uwa.edu.au/research/models/aed/index.html

AED2: dissolved organic carbon - concept



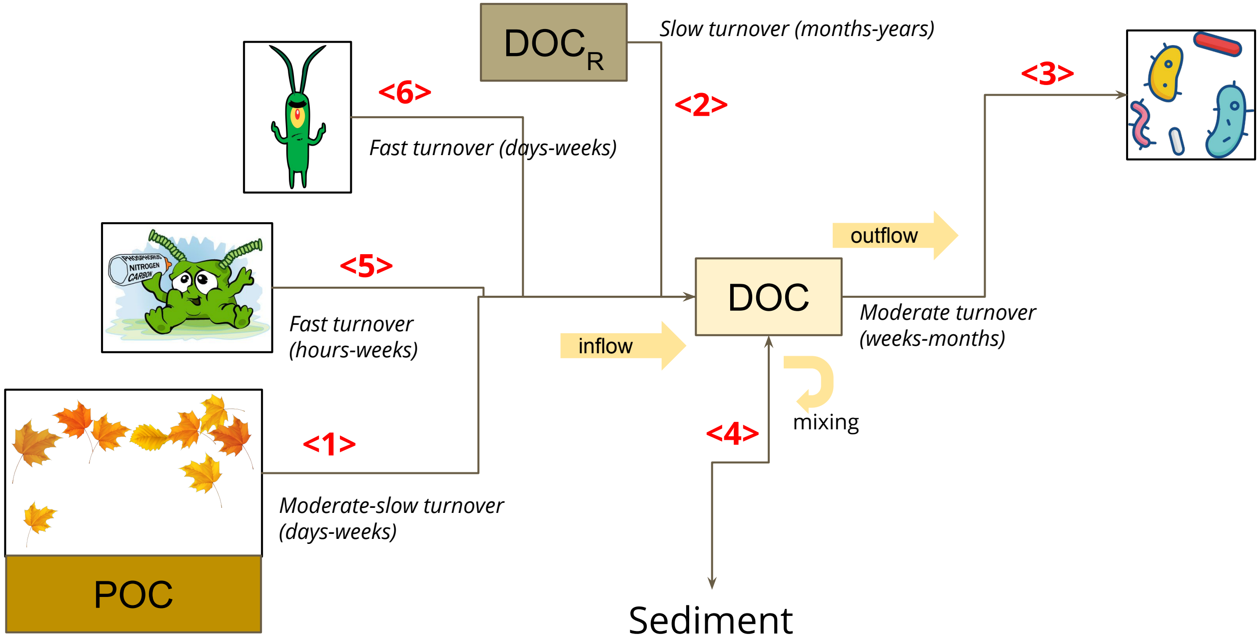
Three pools:

- Labile dissolved OC (**DOC**): fast turnover
- Refractory dissolved OC (**DOCr**): resistant to decomposition
- particulate OC (**POC**)

AED2: dissolved organic carbon - concept

$$\frac{dDOC}{dt} = (1-f_{ref})f^{POC}_{decom} + (1-f_{photo})f^{DOCR}_{photo} - f^{DOC}_{miner} \pm f^{DOC}_{sed} + \sum_{a}^{N_{PHY}} f^{PHY\_C_a}_{excr} + \sum_{z}^{N_{ZOO}} f^{z}_{excr}$$

<1> <2> <3> <4> <5> <6>



- Boxes are variables (states) you can observe
- In the model, C exists only in the boxes
- Arrows are fluxes, transformations, processes you generally cannot observe directly
- Fluxes determine how the boxes change through time
- Fluxes have equations with parameters
- Recalcitrant means the arrow is slow, labile fast
- Fitting a model requires changing parameter values so that boxes match observations, given boundary conditions
- All of these processes happen in all layers

AED2 manual: Hipsey et al. 2013

AED2: dissolved organic carbon - equations

$$\frac{dDOC}{dt} = (1-f_{ref})f_{decom}^{POC} + (1-f_{photo})f_{photo}^{DOCR} - f_{miner}^{DOC} \pm f_{sed}^{DOC} + \sum_{a}^{N_{PHY}} f_{excr}^{PHY\_C_a} + \sum_{z}^{N_{ZOO}} f_{excr}^{z}$$

= + decomposition from particulate detritus (POC)
+ phototransformation of chromophoric DOM (DOC-R)
– mineralisation by bacteria
± sediment flux
– excretion by phytoplankton groups
– excretion by zooplankton groups

$$\frac{dDOC\_R}{dt} = f_{ref}f_{decom}^{POC} - f_{miner}^{DOCR} - f_{photo}^{DOCR} \pm f_{sed}^{DOCR}$$

= + accumulation during particulate detritus (POC) mineralisation
– slow mineralisation by bacteria
– photolysis of chromophoric DOM (DOC-R)
± sediment flux

$$\frac{dPOC}{dt} = f_{bdown}^{CPOM} - f_{decom}^{POC} - f_{sett}^{POC} + \sum_{a}^{N_{PHY}} f_{mort}^{PHY\_C_i} + \sum_{z}^{N_{ZOO}} \left[(1-k_{assim}^{z})f_{assim}^{z} + (1-k_{fsed}^{z})f_{fecal}^{z} + f_{mort}^{z}\right]$$

= + breakdown of CPOM
– decomposition to DOC
± sedimentation
+ mortality from phytoplankton groups
+ messy feeding, faecal pellet release and mortality from zooplankton groups

$$\frac{dCPOM}{dt} = -f_{bdown}^{CPOM} - f_{sett}^{CPOM}$$

= – breakdown of CPOM
± sedimentation

Aerobic mineralization of DOC

f(O2) = scales from 0-1 based on [O2]

f(T) = scales from ~0.2-2.0 based on T

$$f_{miner}^{VAR} = R_{miner}^{VAR} \frac{[O_2]}{K_{miner}+[O_2]} (\theta_{miner})^{T-20} [VAR]$$

(15)

$$+ f_{denit}^{NO_3} \chi_{denit}^{VAR}$$

(16)

Anaerobic mineralization of DOM

RDOC, minimum-maximum rate of aerobic mineralization of labile DOC @20C (0.01-0.10 d^{-1})

AED2 manual: Hipsey et al. 2013, AED2 homepage: https://aed.see.uwa.edu.au/research/models/aed/aed_organic_matter.html

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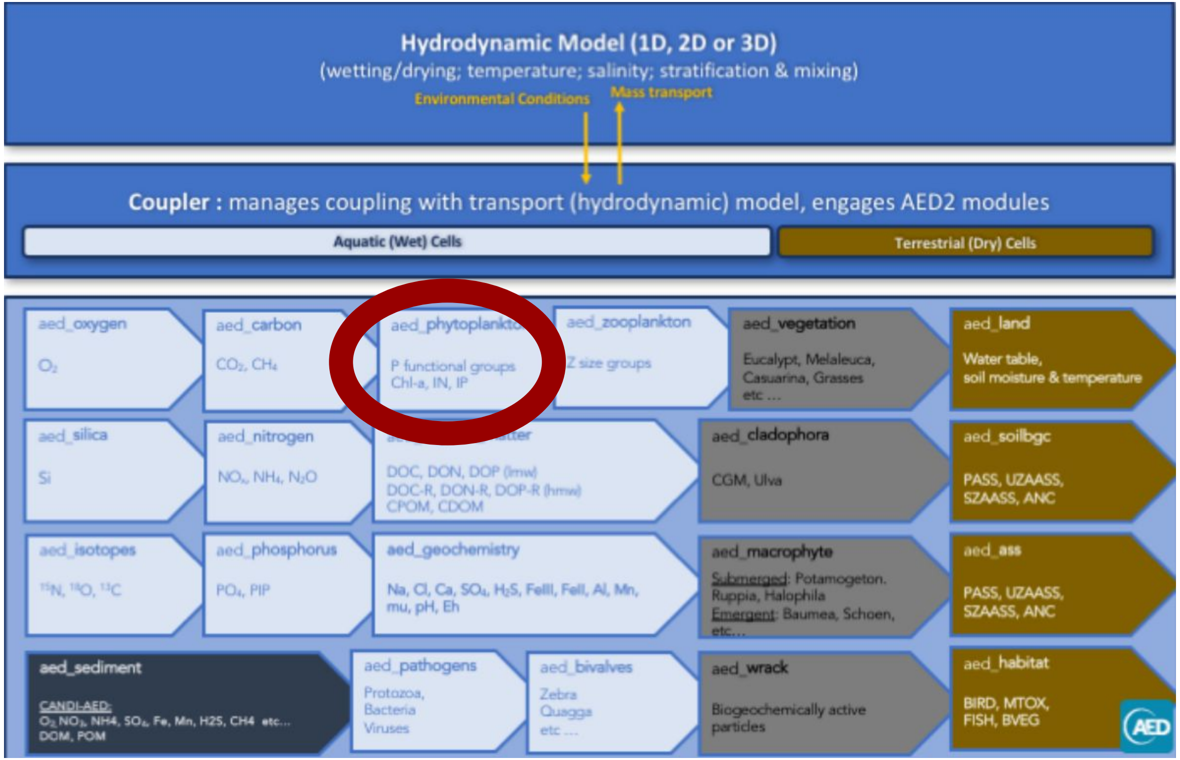
- Hierarchy of dependencies between modules, e.g., nitrogen reactions can depend on availability of oxygen



AED2: phytoplankton

- functional group modeling of phytoplankton groups
- you can define all parameters yourself → domain knowledge
  - database: https://aed.see.uwa.edu.au/research/models/AED/aed2_dbase/db_edit.php
- you can also set up zooplankton dynamics (grazing and feeding)

Carbon

$$\frac{d(PHY_{C_a})}{dt} = +f_{uptake}^{PHY_{C_a}} - f_{excr}^{PHY_{C_a}} - f_{mort}^{PHY_{C_a}} - f_{resp}^{PHY_{C_a}} - f_{sett}^{PHY_{C_a}} - \sum_{z}^{N_{ZOO}} (f_{assim}^{z}\ p_a^z)$$

number of species

aed2.nml

```
&aed2_phytoplankton
   num_phytos = 2
   the_phytos = 1, 2
   settling = 3, 3
   p_excretion_target_variable = 'OGM_dop'
   n_excretion_target_variable = 'OGM_don'
   c_excretion_target_variable = 'OGM_doc'
   si_excretion_target_variable = ''
   p_mortality_target_variable = 'OGM_pop'
   n_mortality_target_variable = 'OGM_pon'
   c_mortality_target_variable = 'OGM_poc'
   si_mortality_target_variable = ''
   p1_uptake_target_variable = 'PHS_frp'
   n1_uptake_target_variable = 'NIT_nit'
   n2_uptake_target_variable = 'NIT_amm'
   si_uptake_target_variable = 'SIL_rsi'
   do_uptake_target_variable = 'OXY_oxy'
   c_uptake_target_variable = 'CAR_dic'
   dbase = 'aed2/aed2_phyto_pars.nml'
   extra_diag = .true.
   min_rho = 900
   max_rho = 1200
```

cyanobacteria and diatoms

aed2_phyto_pars.nml

```
&phyto_data
   pd%p_name = 'cyano','diatom'
   pd%p_initial = 10, 8.4
   pd%p0 = 0.03, 0.03
   pd%w_p = 0, -0.05
   pd%Xcc = 50,50
   pd%R_growth = 5.2, 5.8 !1.2, 2.8
   pd%fT_Method = 1, 1
   pd%theta_growth = 1.08, 1.08
   pd%T_std = 20, 15
   pd%T_opt = 28, 20
   pd%T_max = 35, 32
   pd%lightModel = 0, 0
   pd%I_K = 25, 10
   pd%I_S = 100, 100
   pd%KePHY = 0.005, 0.001
   pd%f_pr = 0.005, 0.002
   pd%R_resp = 0.08, 0.12
   pd%theta_resp = 1.05, 1.07
   pd%k_fres = 0.6, 0.6
   pd%k_fdom = 0.05, 0.05
   pd%salTol = 0, 0
   pd%S_bep = 2, 2
   pd%S_maxsp = 35, 35
   pd%S_opt = 1, 1
```

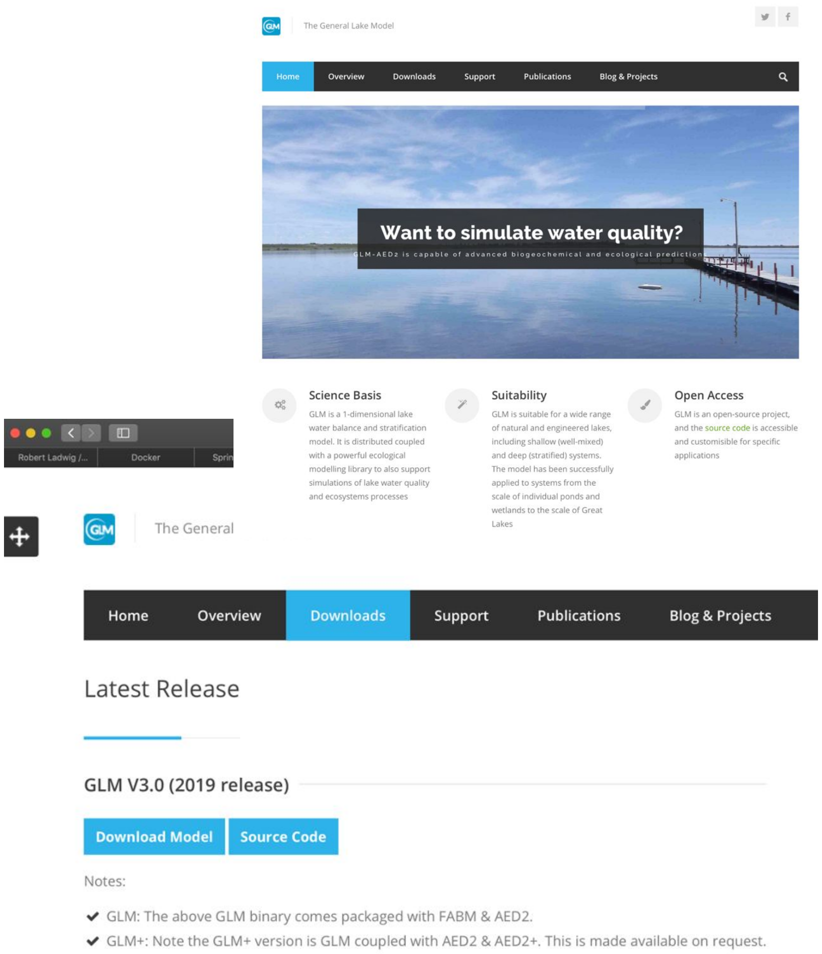
all interactions

parameter file

The General Lake Model (GLM) d: run the model

Setting up GLM

- Installing GLM:
    - Download software package via AED GLM website: http://aed.see.uwa.edu.au/research/models/GLM/latest_release.html (precompiled binaries)
    - Source code and compilation instructions are available, accessible via the GitHub repository - https://github.com/AquaticEcoDynamics/GLM
    - GLM3r in R devtools::install_github("GLEON/GLM3r")



GLM homepage: https://aed.see.uwa.edu.au/research/models/GLM/index.html

Setting up GLM

- Main file: glm3.nml
- Ordered into blocks
  - Begin with: &
  - End with: /
- Includes model setup and relative paths to water quality and driver data
- GLM executable needs the setup file

```
!-------------------------------------------------------------------------------
! general model setup
!-------------------------------------------------------------------------------
&glm_setup
   sim_name = 'Mendota'
   max_layers = 75
   min_layer_vol = 0.1
   min_layer_thick = 0.15
   max_layer_thick = 1.5
   density_model = 1
/
&mixing
   surface_mixing = 1
   coef_mix_conv = 0.2
   coef_wind_stir = 0.23
   coef_mix_shear = 0.3
   coef_mix_turb = 0.51
   coef_mix_KH = 0.3
   coef_mix_hyp = 0.4689587
   deep_mixing = 2
   diff = 0
/
&light
   light_mode = 0
   n_bands = 4
   light_extc = 1, 0.5, 2, 4
   energy_frac = 0.51, 0.45, 0.035, 0.005
   Benthic_Imin = 10
   Kw = 0.4315141
/
!-------------------------------------------------------------------------------
! water quality setup
! if this block is read, water quality functionality will be enabled
!-------------------------------------------------------------------------------
```

GLM homepage: https://aed.see.uwa.edu.au/research/models/GLM/index.html

Setting up GLM

- Define the &morphometry
  - Area-depth relationship (&H and &A)
- Define what you want to simulate
  - State variables (temperature, salinity, etc.)
  - Grid resolution and time step (&glm_setup, &time)
- Define external environment
  - Boundary conditions (inflows, meteorology, outflows) (&meteorology, &inflows, &outflows)
- Provide an initial condition (&init_profiles)
- Start your simulation

glm3.nml file

&glm_setup:	General simulation info
&wq_setup:	Water quality
&time:	Time control
&morphometry:	Lake morphometric information
&output:	Output file details
&init_profiles:	Initial vertical profiles
&meteorology:	Surface forcing and meeorology
&inflows:	Information about inflowing rivers
&outflows:	Information about outflows
&light:	Information about light climate

GLM homepage: https://aed.see.uwa.edu.au/research/models/GLM/index.html

Setting up GLM

- Boundary conditions: data that drive the model
- At minimum, GLM needs meteorological data (hourly or daily) in CSV-format

```
Date,ShortWave,LongWave,AirTemp,RelHum,WindSpeed,Rain,Snow
2009-01-01 00:00:00,0,191.50999,-15.609991,88.86569,2.9134343,0,0
2009-01-01 01:00:00,0,217.56,-14.750006,88.178638,3.5679266,0,0
2009-01-01 02:00:00,0,217.56,-14.15,88.305945,3.9796608,0,0
2009-01-01 03:00:00,0,217.57001,-13.560004,88.286784,4.3862171,0,0
2009-01-01 04:00:00,0,230.42999,-12.959998,88.028059,4.8016873,0,0
2009-01-01 05:00:00,0,230.42999,-12.449988,87.745015,5.3791169,0,0
2009-01-01 06:00:00,0,230.42999,-11.929999,87.288882,5.9664732,0,0
2009-01-01 07:00:00,0,246.75,-11.41001,86.734669,6.5488395,0,0
2009-01-01 08:00:00,0,246.75999,-10.620001,86.510658,6.995177,0,0
2009-01-01 09:00:00,50.312,246.75999,-9.8200134,85.935506,7.4708298,0,0
2009-01-01 10:00:00,168.256,253.35001,-9.0199951,85.14882,7.9805386,0,0
2009-01-01 11:00:00,255.60001,253.35001,-7.8599915,85.236462,8.1806115,0,0
2009-01-01 12:00:00,325.892,253.35001,-6.6900085,84.658597,8.4221193,0,0
2009-01-01 13:00:00,349.651,265.15002,-5.5300049,83.680197,8.6924564,0,0
2009-01-01 14:00:00,318.17099,265.14999,-4.9799866,84.281007,8.1392691,0,0
2009-01-01 15:00:00,264.33701,265.14999,-4.4299988,84.709775,7.6592037,0,0
2009-01-01 16:00:00,153.472,271.73001,-3.880011,84.970459,7.2817926,0,0
2009-01-01 17:00:00,51.591999,271.73001,-4.1399902,86.532806,6.6806363,0,0
```

```
Time,FLOW,TEMP,SALT
2009-01-01 00:00:00,3.560861,-0.526716,0
2009-01-02 00:00:00,6.162997,-0.585426,0
2009-01-03 00:00:00,3.826635,-0.639793,0
2009-01-04 00:00:00,5.397271,-0.696168,0
2009-01-05 00:00:00,5.417987,-0.742644,0
2009-01-06 00:00:00,3.886593,-0.784772,0
2009-01-07 00:00:00,5.806259,-0.821455,0
2009-01-08 00:00:00,5.65432,-0.85336,0
2009-01-09 00:00:00,4.725836,-0.873803,0
2009-01-10 00:00:00,5.821722,-0.906718,0
2009-01-11 00:00:00,5.724123,-0.926215,0
2009-01-12 00:00:00,5.495776,-0.936452,0
2009-01-13 00:00:00,5.473368,-0.947798,0
2009-01-14 00:00:00,5.513825,-0.955154,0
```

- And flow data (inflow and/or outflow, hourly or daily) in CSV-format

GLM homepage: https://aed.see.uwa.edu.au/research/models/GLM/index.html

Setting up GLM: buildyourownmodel/

Your first steps:

(1) Download meteorological data of your site: *radiation, wind speed, air temperature, rainfall, relative humidity*

(2) use toy glm3.nml file in workshop material to

  (a) insert lake hypsography

  (b) relative path to meteorological driver data file (CSV)

(3) run lake model in R, see 'run_GLMmodel.R'

Let's switch

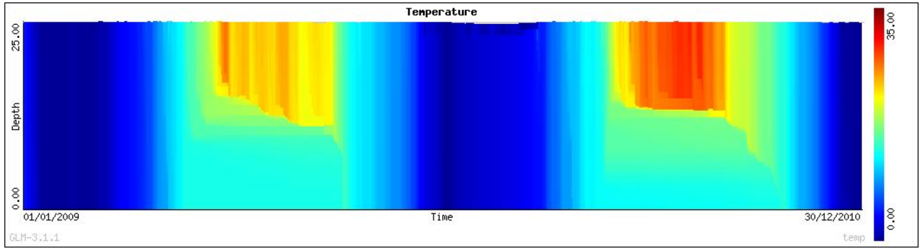
Setting up GLM: buildyourownmodel/

Your first steps:

(1) Download meteorological data of your site: *radiation, wind speed, air temperature, rainfall, relative humidity*

(2) use toy glm3.nml file in workshop material to
   (a) insert lake hypsography
   (b) relative path to meteorological driver data file (CSV)

(3) run lake model in R, see ‘run_GLMmodel.R’



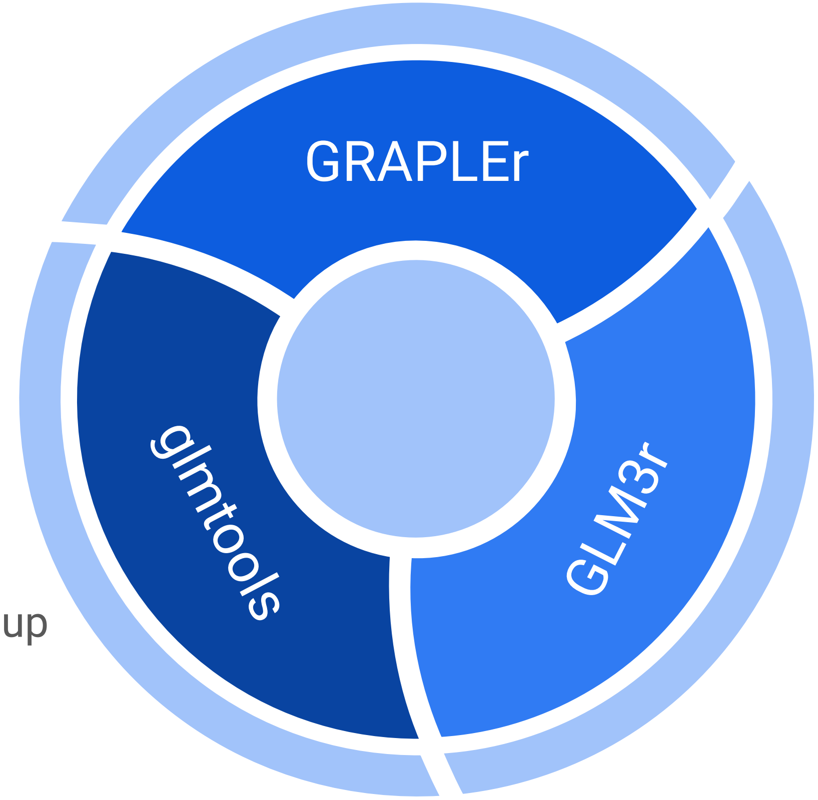
What you get:

(1) output.nc - all output variables
(2) lake.csv - daily diagnostics
(3) abovesediment*.csv - output at specific depths
(4) heatmap plot - temperature output

GLM homepage: https://aed.see.uwa.edu.au/research/models/GLM/index.html

GLM in R

- Distributed computing system
- Run multiple GLM simulations



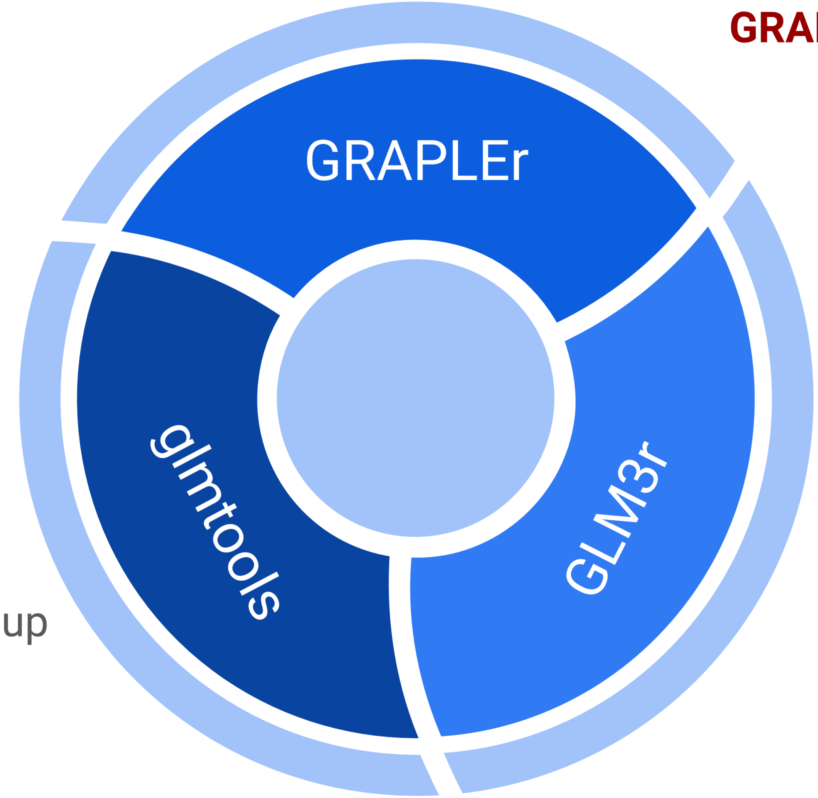
- Run GLM in R

- Changing model setup
- Visualizing results
- Physical derivatives
- Calibration

GLM in R

- Distributed computing system
- Run multiple GLM simulations

GRAPLE/GRAPLEr



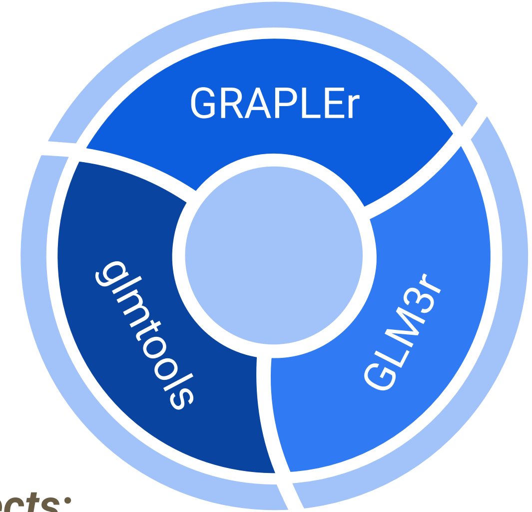
USGS-R/glmtools

- Changing model setup
- Visualizing results
- Physical derivatives
- Calibration

GLEON/GLM3r

- Run GLM in R

GLM in R



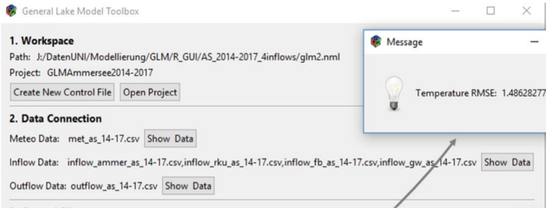
More awesome R-related GLM projects:

Macrosystems EDDIE: classroom modules to teach macrosystems ecology

LakeEnsemblR: R-package to run lake ensembles

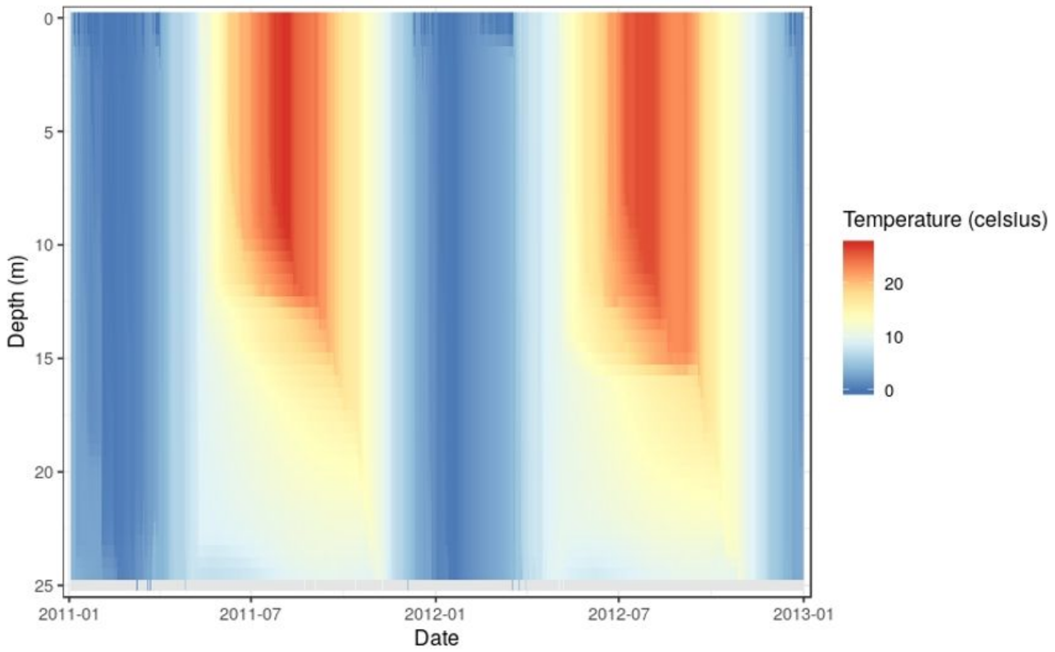
glmGUI: GUI and toolbox to run GLM

Columbus4Limnology: Run GLM online in the cloud (release soon)



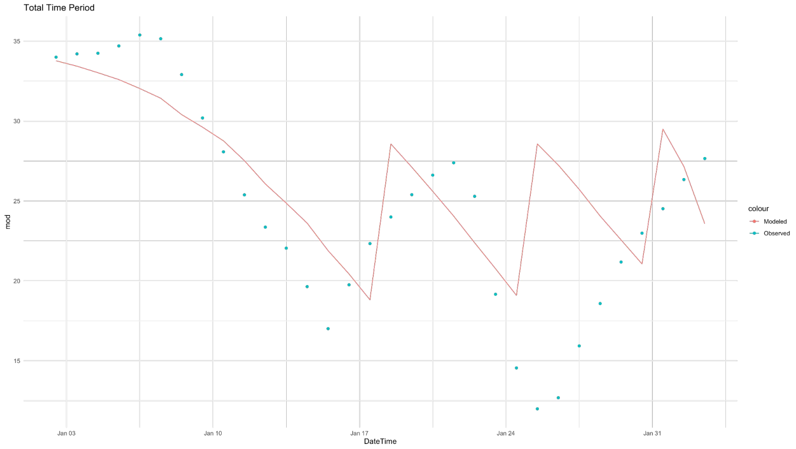
glmtools

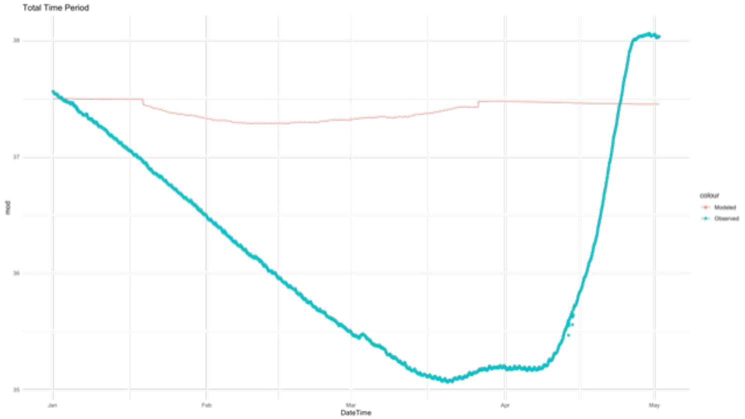
- Either from github or GRAN
- Offers lots of functionalities:
  - Manipulate model setup
  - Retrieve output data
  - Compare observed to simulated data
  - Visualize results
  - Calibration functions
- ‘ggplot_overhaul’ branch includes up-to-date version with experimental features (e.g., water quality calibration)



glmtools

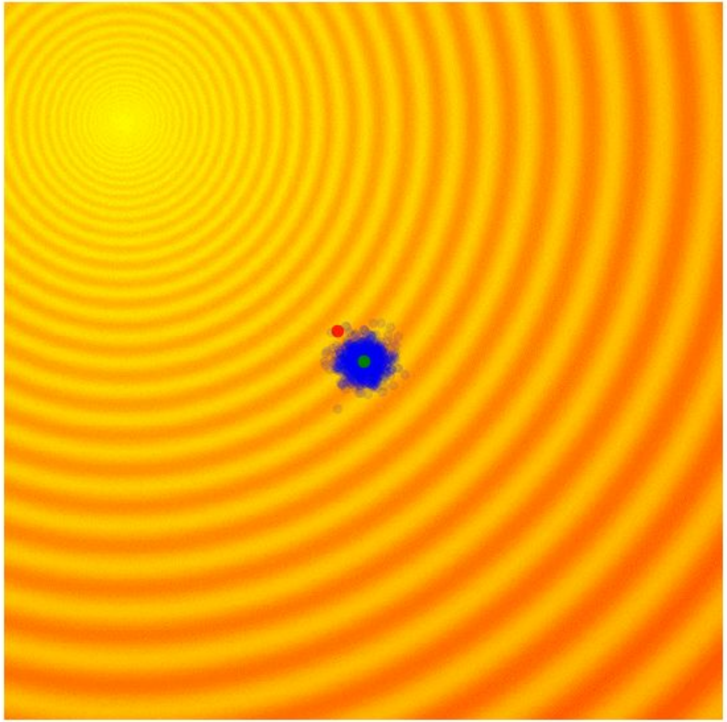
- experimental version available at https://github.com/robertladwig/glmtools/tree/ggplot_overhaul
- small bug fixes
- calibration functions for water level (reservoir management, closing water balance, …)
    - can reveal missing inflows or outflows
    - can identify missing ice formation





glmtools: calibration

a) CMA-ES: derivative-free optimization, which adaptively changes the search path for every generation (modifying normal distribution and covariance matrix), covers wide search space, converges fast but needs more computational time (~O(N2))
b) Nelder-Mead method: derivative-free optimization, direct search method



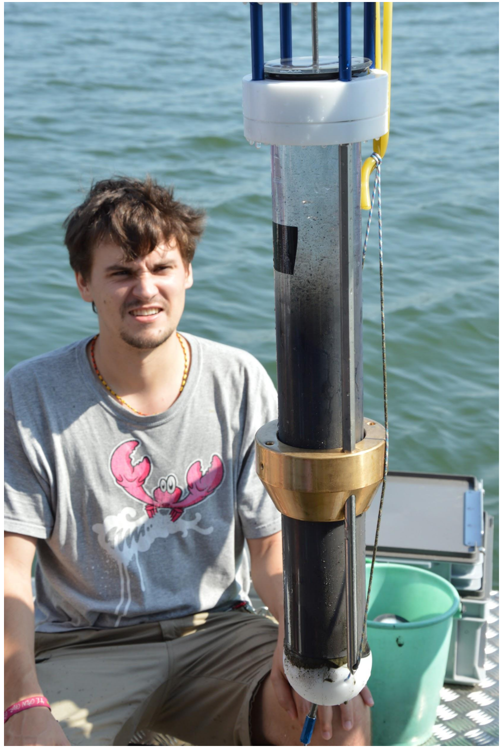
Github: https://github.com/USGS-R/glmtools, CMA-ES algorithm: Hansen 2006, animation by https://blog.otoro.net

Learn from the expert: *Ensemble modeling of lake phenology changes*

J. Feldbauer, T.N. Moore, J. Mesman, R. Ladwig, T. Berendonk, H. Zündorf, and T. Petzoldt: Ensemble of models show coherent response of a reservoir's stratification and ice cover to climate warming, *submitted to Aquatic Sciences*

- application of LakeEnsemblR running FLake, GLM, GOTM, Simstrat and MyLake on a German reservoir

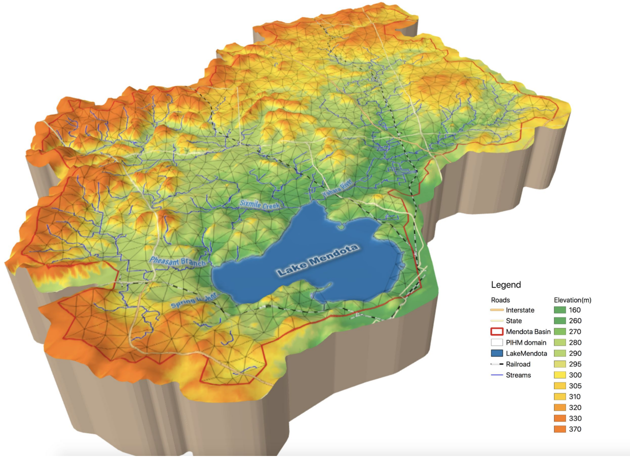
LakeEnsemblR

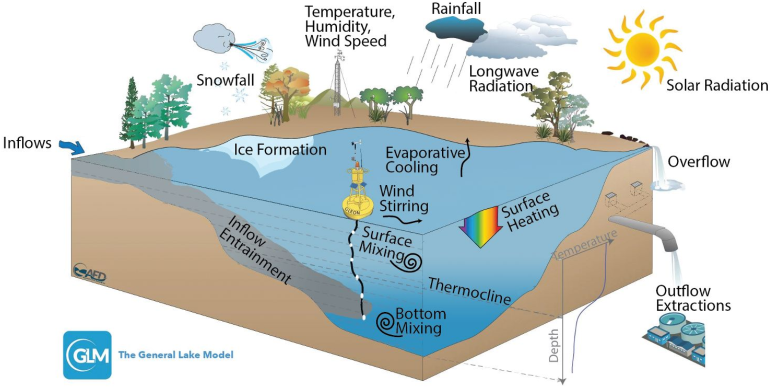


Hands-on exercises

Lake Mendota in Wisconsin, USA

- **Lake Mendota**: eutrophic, 25 m max. depth, residence time ~ 4-5 years
- 70 % agricultural and 25 % urban watershed
- dimictic: strong summer stratification with cyanobacteria bloom, ice formation during winter





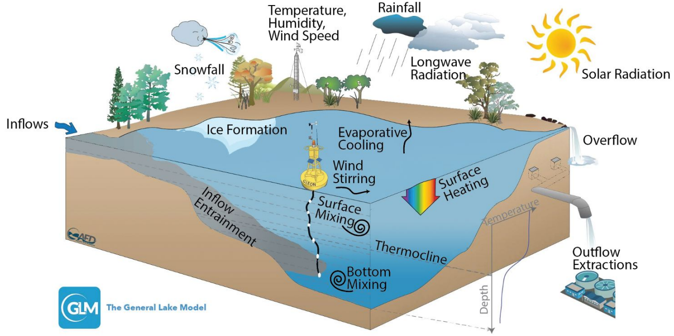
Lake Mendota in Wisconsin, USA

Example 1: reading the configuration file into R

Example 2: model output processing and visualizations

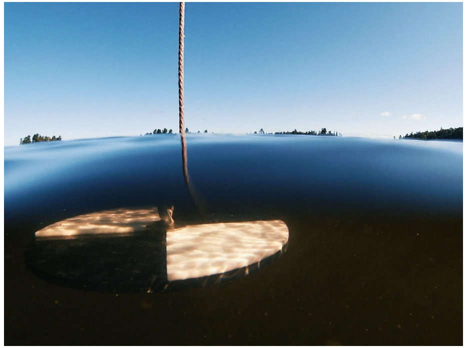
Example 3: calibrating water temperature parameters

Example 4: calibrating dissolved oxygen parameters



Example 5a: Team *Physics* (climate change impact on lake ice)

Example 5b: Team *Biology* (nutrients driving algae blooms)



(bonus) Example 6: check your phytoplankton dynamics

ice picture by Clean Lakes Alliance, Secchi disk image by Hilary Dugan @hildug

Let's switch

Wrapping up

Questions, issues, problems & feedback?

Thank you for joining!

Have fun lake modeling!

Join the GLM Slack for help and support: https://join.slack.com/t/general-lake-model/shared_invite/zt-a7pyrxhj-oe4dYm6oLQfk1r_ZGLFTwQ

Interested in lake modeling? Join our working group meetings this week https://gleon.org/research/working-groups/ecosystem-modeling