



# Process-based lake modeling in R using GLM (General Lake Model)

Experiment on your lakes safely from home on your laptop

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# Who's who?

Robert, postdoc at  
Center for Limnology



Hilary, Assistant Prof.  
UW-Madison



Aryan, undergrad in  
Computer Science



Paul, Research Prof.  
UW-Madison

# 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!
- Future questions? Email Robert at [rladwig2@wisc.edu](mailto:rladwig2@wisc.edu)

Two paths to do the [workshop examples](#):

- (1) Clone and download files from: [https://github.com/robertladwig/GLM\\_workshop](https://github.com/robertladwig/GLM_workshop)
  - (a) you'll need R (>= 3.5) and these packages: GLM3r, glmtools, rLakeAnalyzer, tidyverse, reshape2, lubridate, pracma (instructions are online)
- (2) Use the docker: <https://hub.docker.com/r/hydrobert/glm-workshop> (requires docker)
  - (a) this includes Rocker, all packages, all scripts and all data; then open a terminal:

```
docker pull hydrobert/glm-workshop
```

```
docker run -rm -d -p 8000:8000 -e ROOT=TRUE -e PASSWORD=password hydrobert/glm-workshop:latest
```

open any web browser and type 'localhost:8000' (user: rstudio, password: password)

# Time schedule today

9:30-10:20	<b>Introduction to process-based lake modeling</b>	<ul style="list-style-type: none"><li>• What is process-based modeling?</li><li>• GLM theory and applications</li><li>• AED2 theory and examples for O<sub>2</sub> and C</li><li>• Overview of R-packages</li></ul>
10:25-11:15	<b>Using the model in R</b>	<ul style="list-style-type: none"><li>• Running GLM in R</li><li>• Visualising results</li><li>• Calibrating water temp. and oxygen parameters</li><li>• Checking your phytoplankton</li></ul>
11:15-11:30	<b>Questions and problems</b>	<ul style="list-style-type: none"><li>• Stick around to talk about questions and raise issues</li></ul>

# Time schedule today

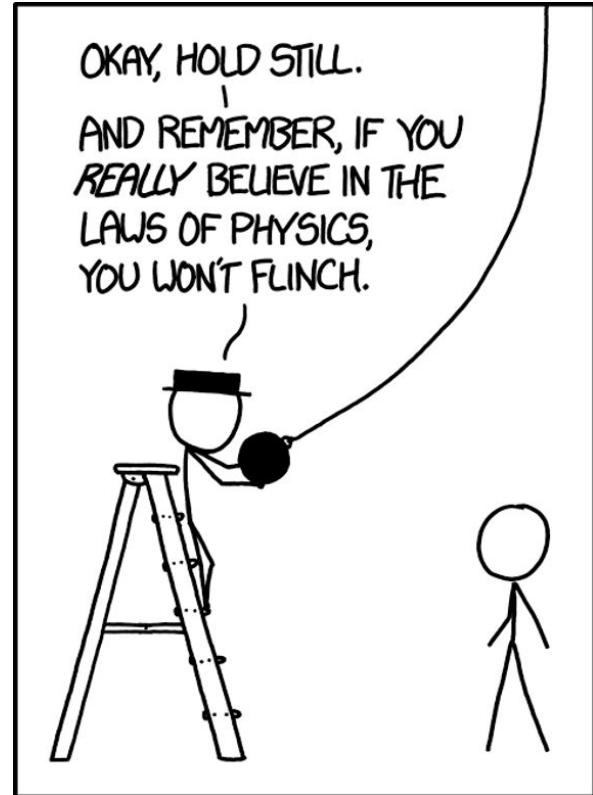
9:30-10:15	Introduction to process-based lake modeling	<ul style="list-style-type: none"><li>• What is process-based modeling?</li><li>• GLM theory</li><li>• AED2 theory</li><li>• Overview of the model</li></ul>
10:30-11:15	Using the model in R	<ul style="list-style-type: none"><li>• Running the model</li><li>• Visualizing results</li><li>• Calibration</li><li>• Checking results</li></ul>
11:15-11:30	Questions and problems	<ul style="list-style-type: none"><li>• Stick around to ask questions!</li></ul>

Please ask urgent questions by "raising hand" in Zoom;  
Otherwise you can write your question/issue [here](#) and we will talk about it at the end

# Modeling introduction

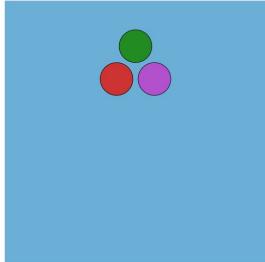
# Process-based modeling in a nutshell

- 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)



# Process-based modeling in a nutshell

- **Conservation of mass (continuity)**
  - Inflow(s)= outflow(s)
  - Mass cannot be created or destroyed
- **Conservation of momentum**
  - Velocity based on balances of forces (gravity, pressure, friction, earth-rotation)



State of the environment



$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = q_0$$
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + g + \nu \Delta \mathbf{v}$$



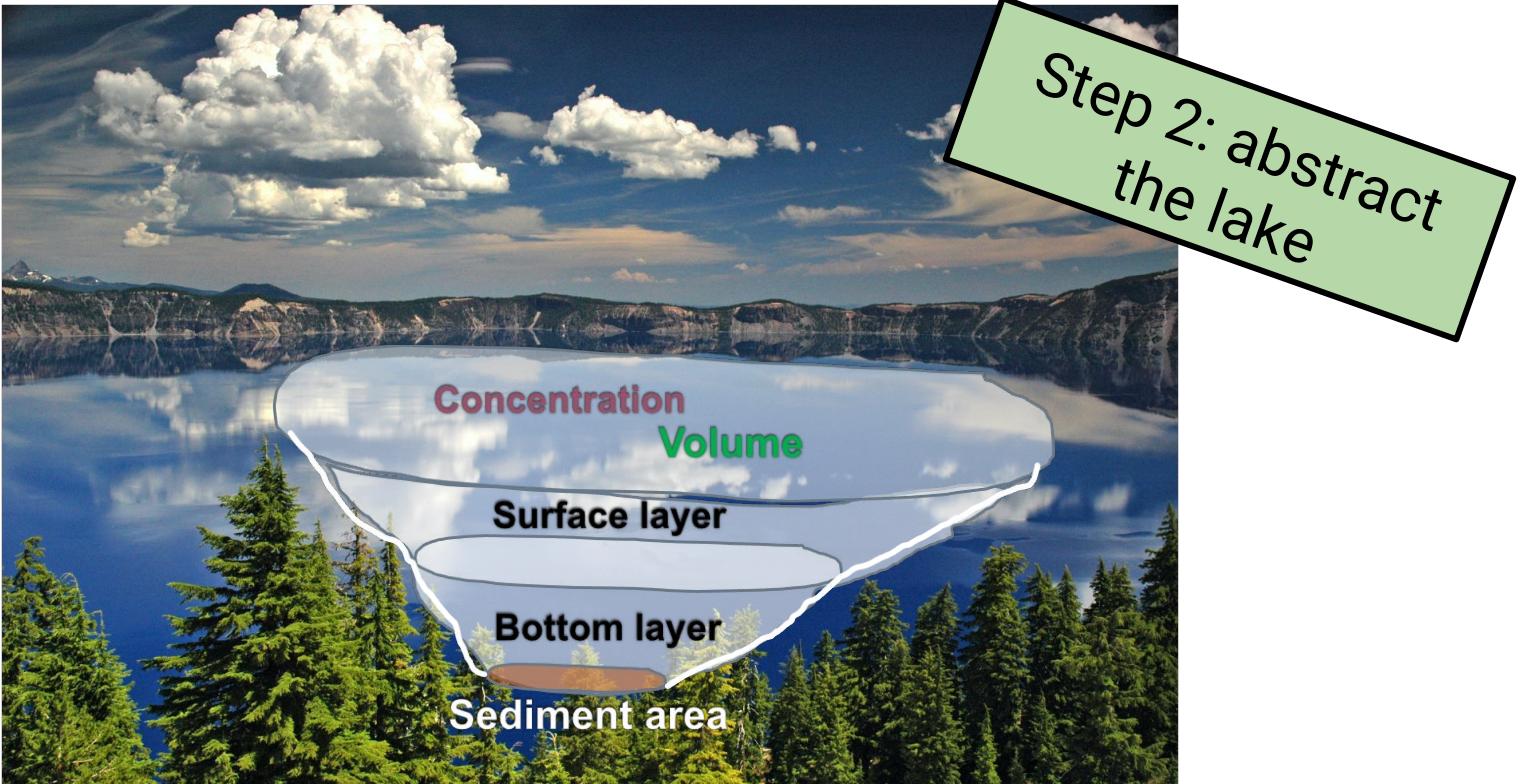
State of the system

# Process-based modeling in a nutshell

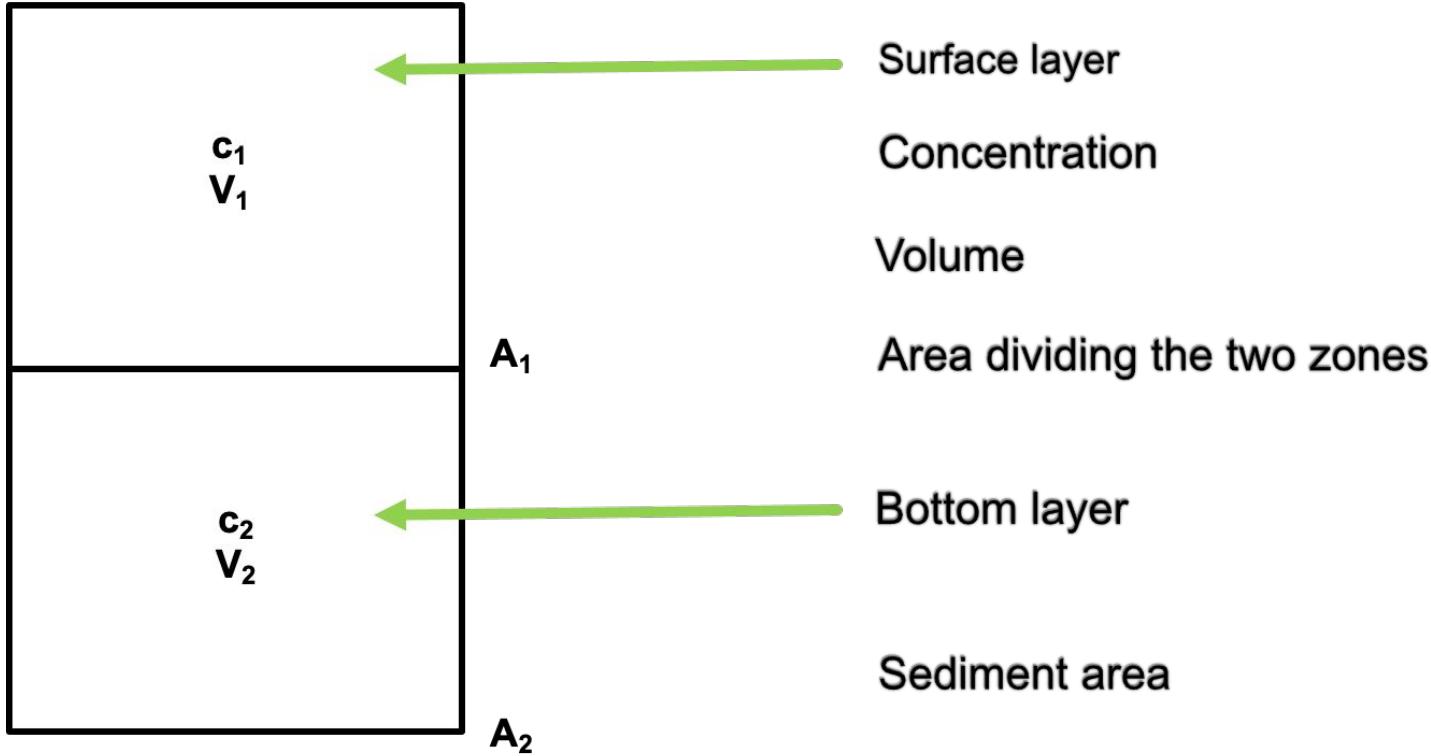


*Step 1: imagine a  
(nice) lake*

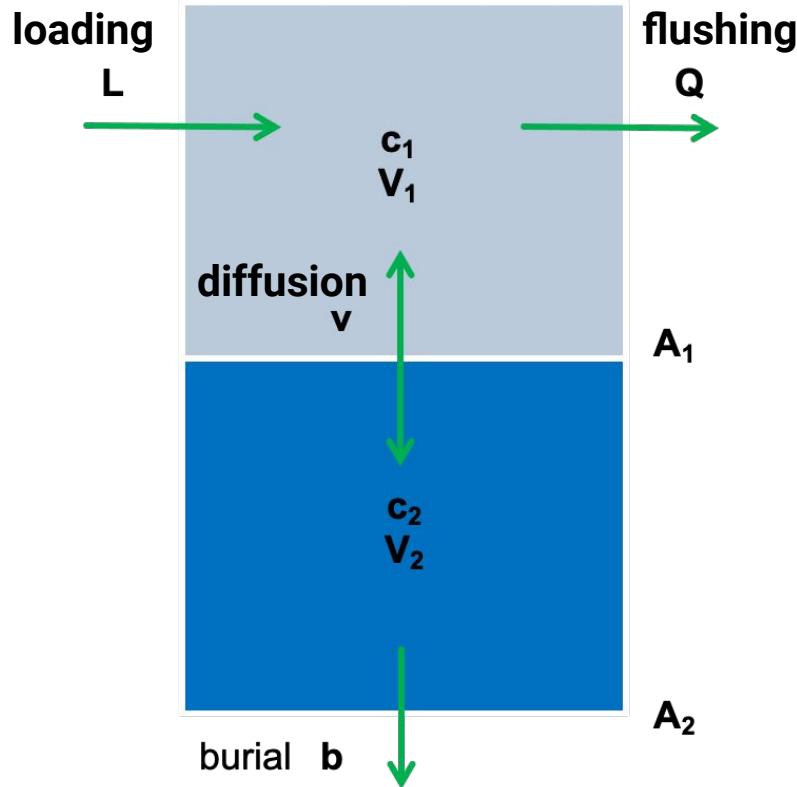
# Process-based modeling in a nutshell



# Process-based modeling in a nutshell



# Process-based modeling in a nutshell

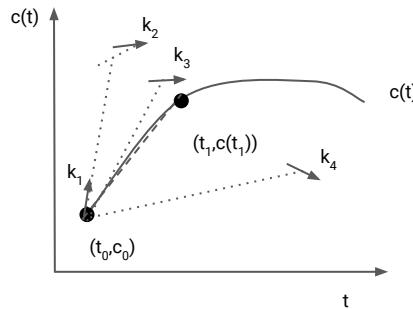
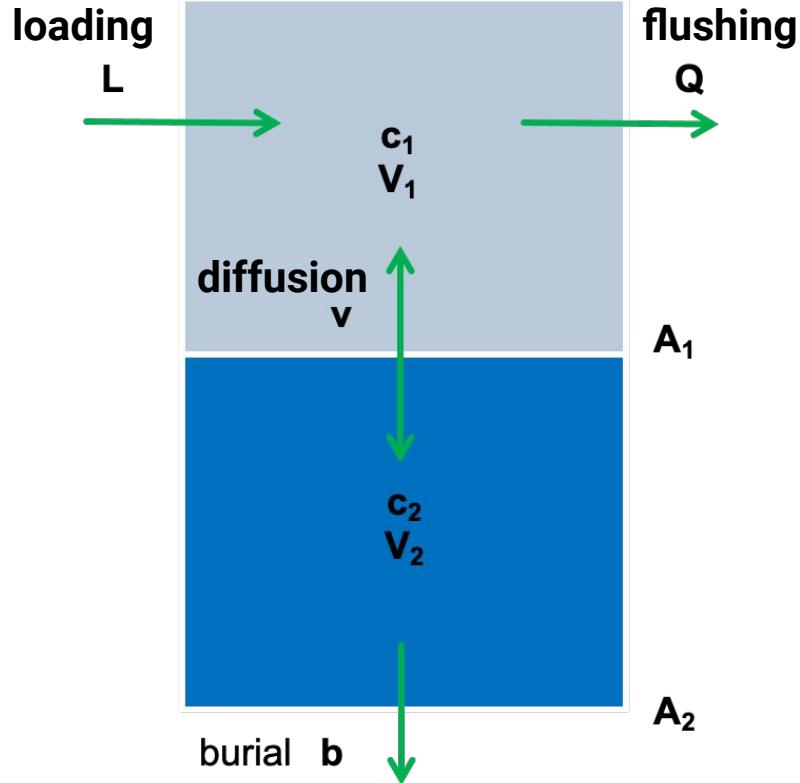


Step 3: add math

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

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

# Process-based modeling in a nutshell

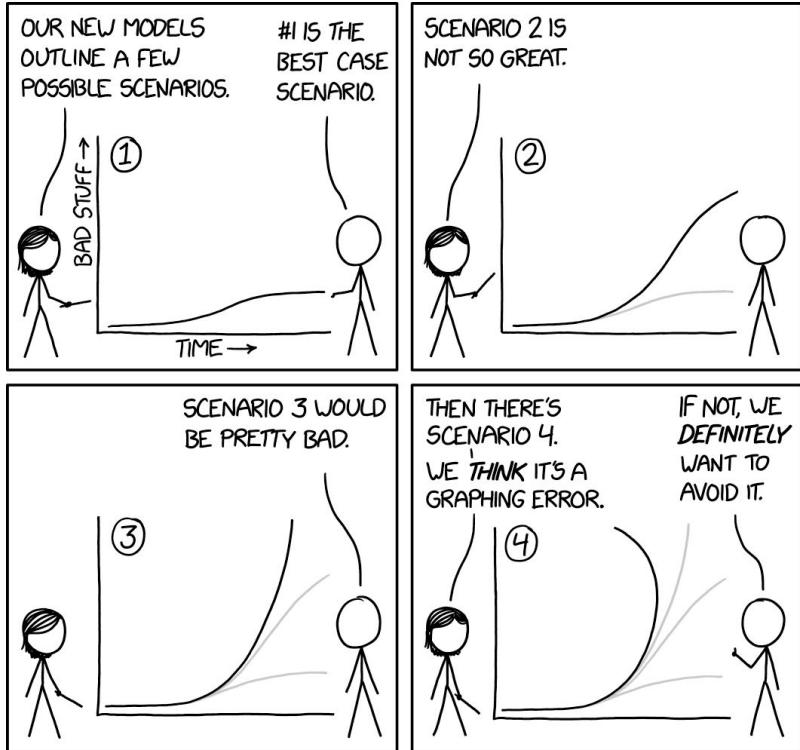


*Step 4: solve with numerics, e.g., Runge-Kutta*

$$\begin{aligned}
 c_{i+1} &= c_i + f(c_i, t_i) * \Delta t \quad h = \Delta t \\
 c_{i+1} &= c_i + [\frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)]\Delta t \\
 k_1 &= f(t_i, c_i) \\
 k_2 &= f(t_i + \frac{1}{2}h, c_i + \frac{1}{2}hk_1) \\
 k_3 &= f(t_i + \frac{1}{2}h, c_i + \frac{1}{2}hk_2) \\
 k_4 &= f(t_i + h, c_i + hk_3)
 \end{aligned}$$

# Process-based modeling in a nutshell

- Why should you use a model?
- Explore ideas regarding ecological systems that may not be possible/feasible to field-test for
  - logistical reasons
  - political reasons
  - financial reasons
  - physical reasons
- Formulating a model helps to better understand the system and can identify data needs
- “Your model is your hypothesis.” ([Kate](#))

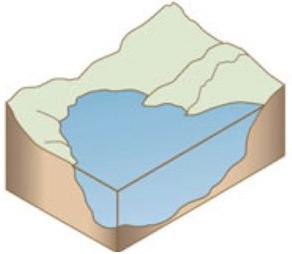


# GLM

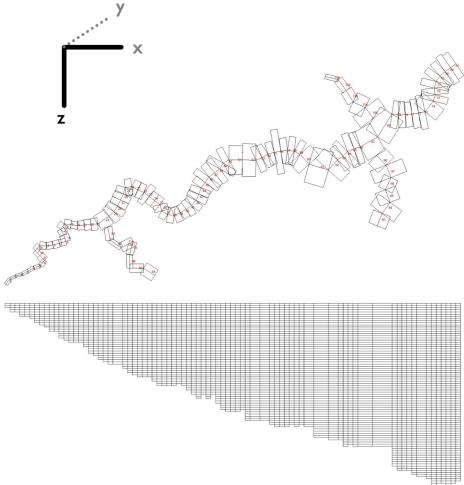
# introduction

# Multi-dimensional models

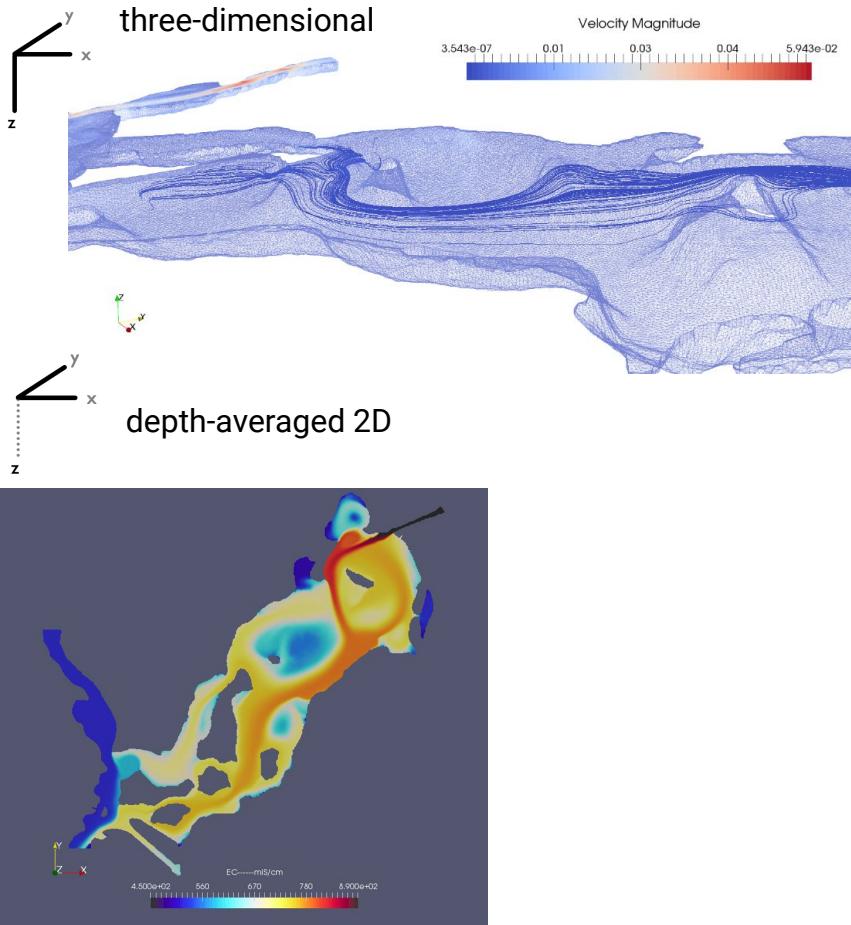
zero-dimensional  
0D: Box model



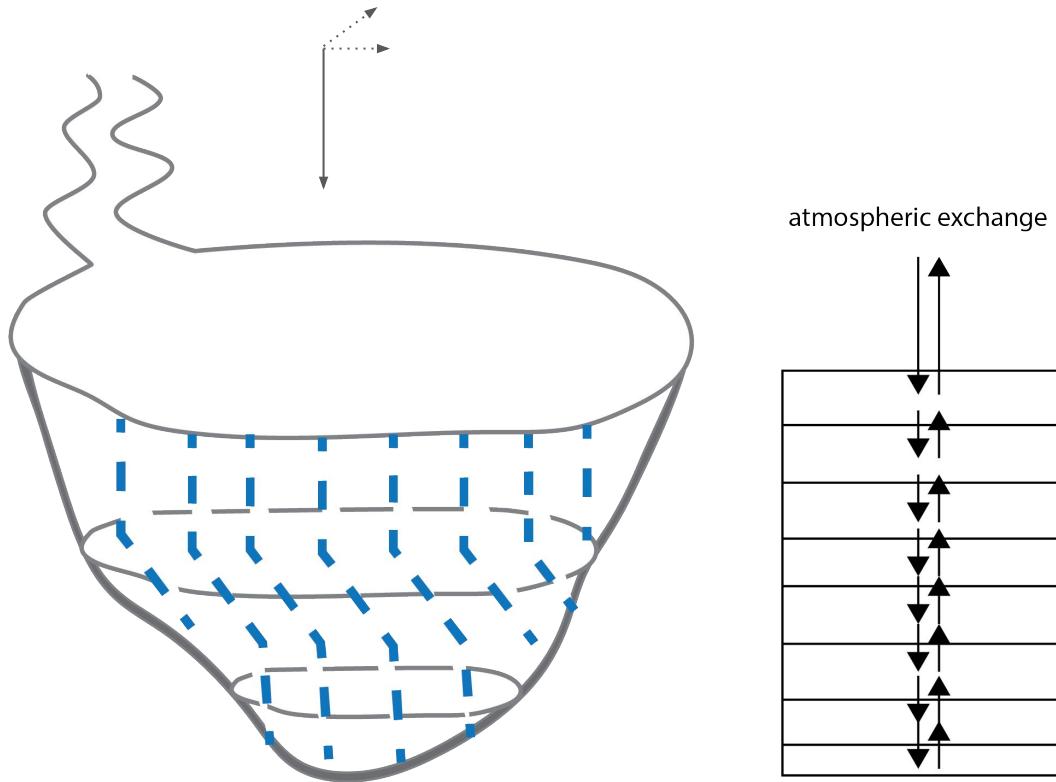
longitudinal-vertical 2D



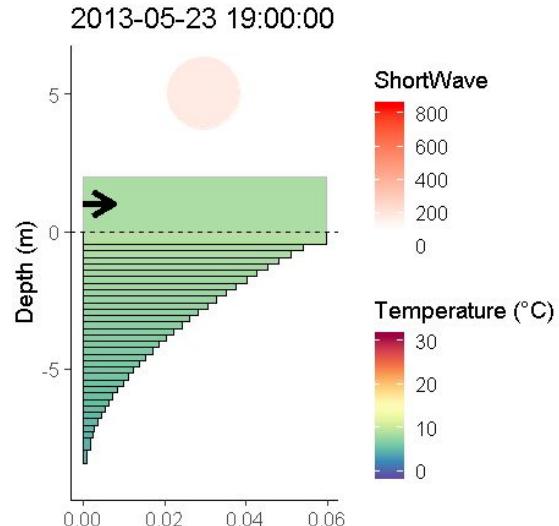
0D model: Trolle et al. 2012; longitudinal-vertical 2D model: Mi et al. 2020



# 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**



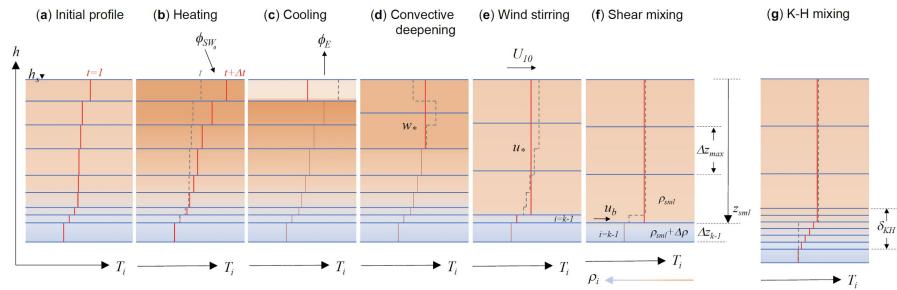
# Process-based lake modeling

- Reactive-diffusive transport equation for water temperature
- Turbulence-closure scheme to solve for momentum terms and diffusivities (e.g., k- $\epsilon$  in Simstrat)
- Molecular diffusivity is mostly neglected → approximation of  $K_z$  (e.g., MyLake)
- Alternatively, energy-balance approaches (e.g., GLM): potential ag. available kinetic energy

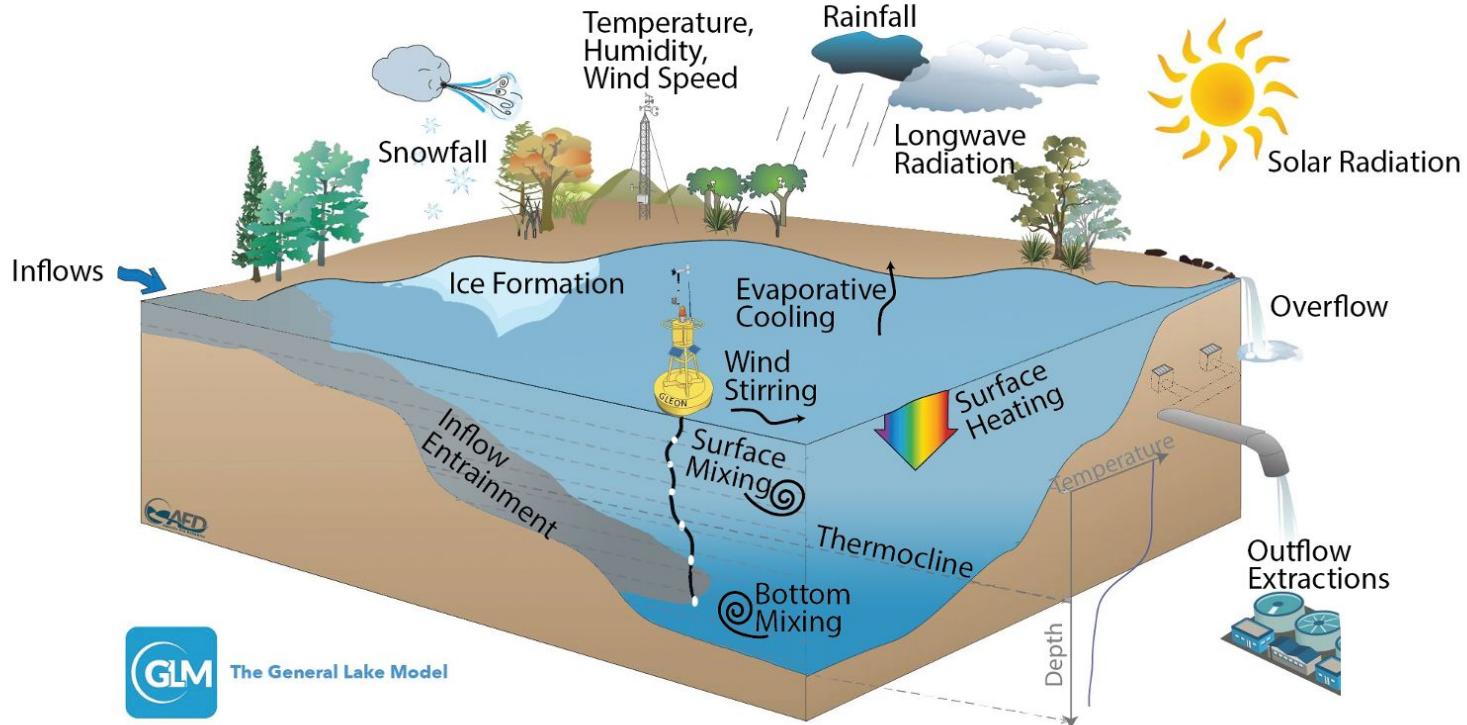
$$\frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial z} \left( A(v_t^c + v^i) \frac{\partial T}{\partial z} \right) + \frac{1}{\rho_0 c_p} \frac{\partial H_{sol}}{\partial z} + \frac{dA}{dz} \frac{H_{geo}}{A \rho_0 c_p}$$

diffusive transport      atmospheric heating      sediment heating

$$\frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial z} \left( A K_z \frac{\partial T}{\partial z} \right) + \frac{1}{\rho_0 c_p} \frac{\partial H_{sol}}{\partial z}$$

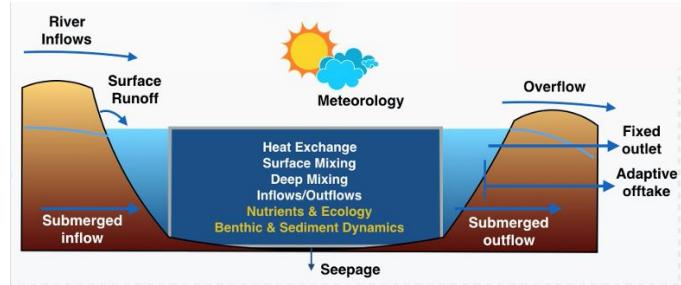


# General Lake Model (GLM)



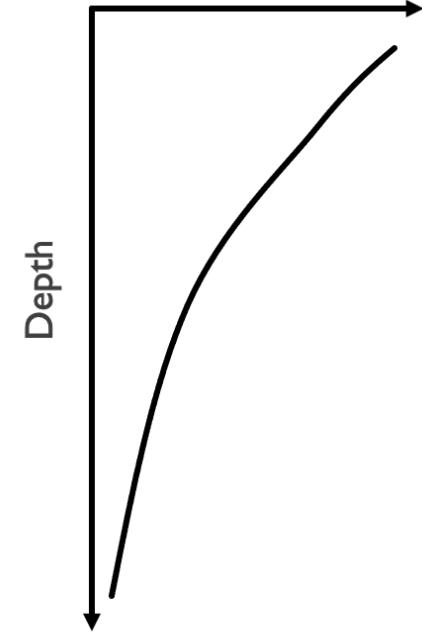
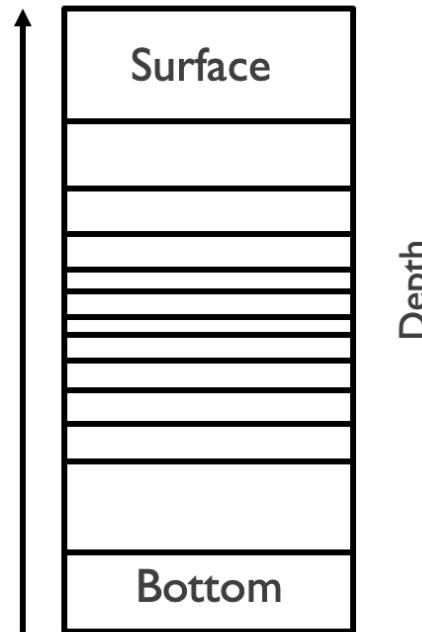
# General Lake Model (GLM)

- 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 (AED) → water quality model
- Written in C and Fortran
- Freely available as open-source program:  
<https://github.com/AquaticEcoDynamics/GLM>



# 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



# Water balance

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

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

## Surface layer height

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

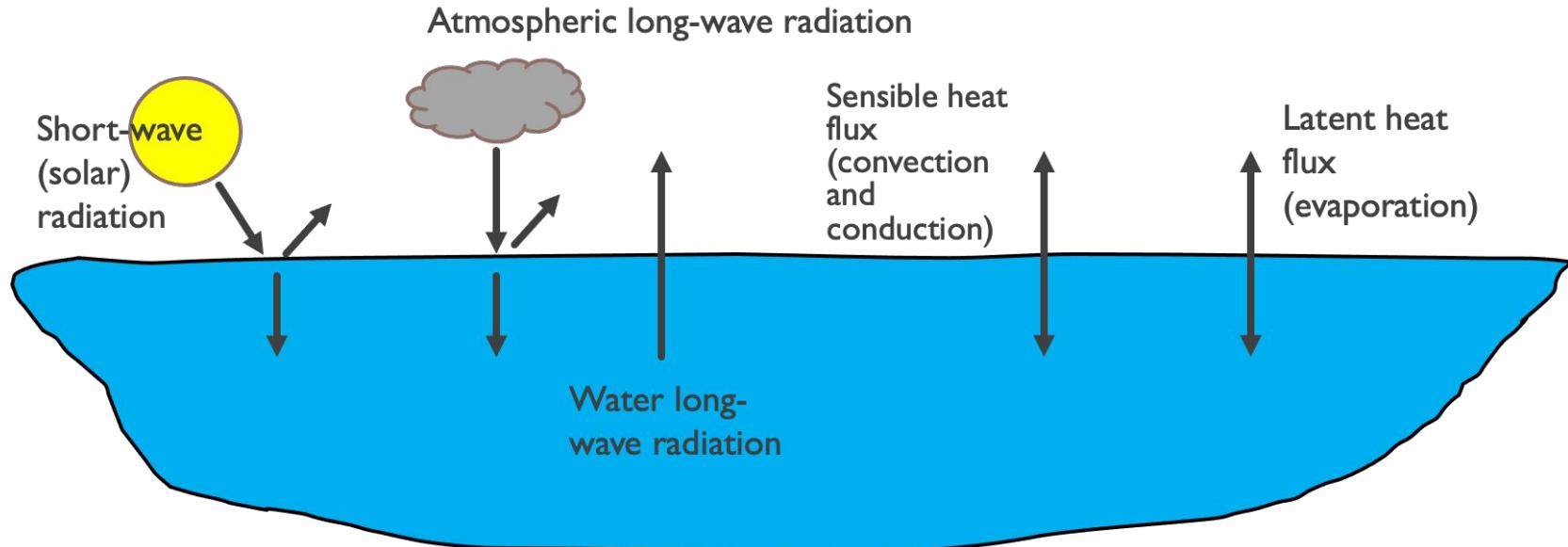
Mass balance of surface layer = precipitation + snowfall + run-off – evaporation - ice

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

- Mixing only affects thickness of surface layer ( $z_{sml}$ ) not its height

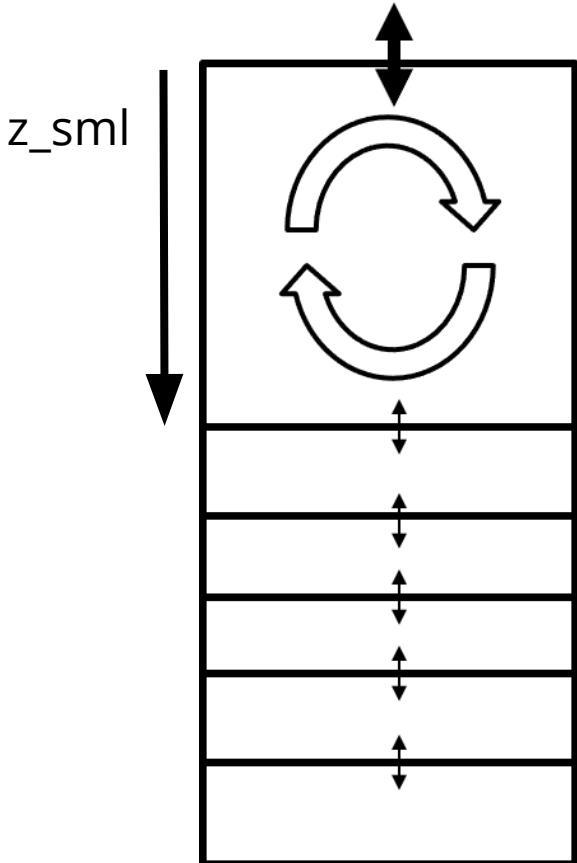
# Surface energy balance

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

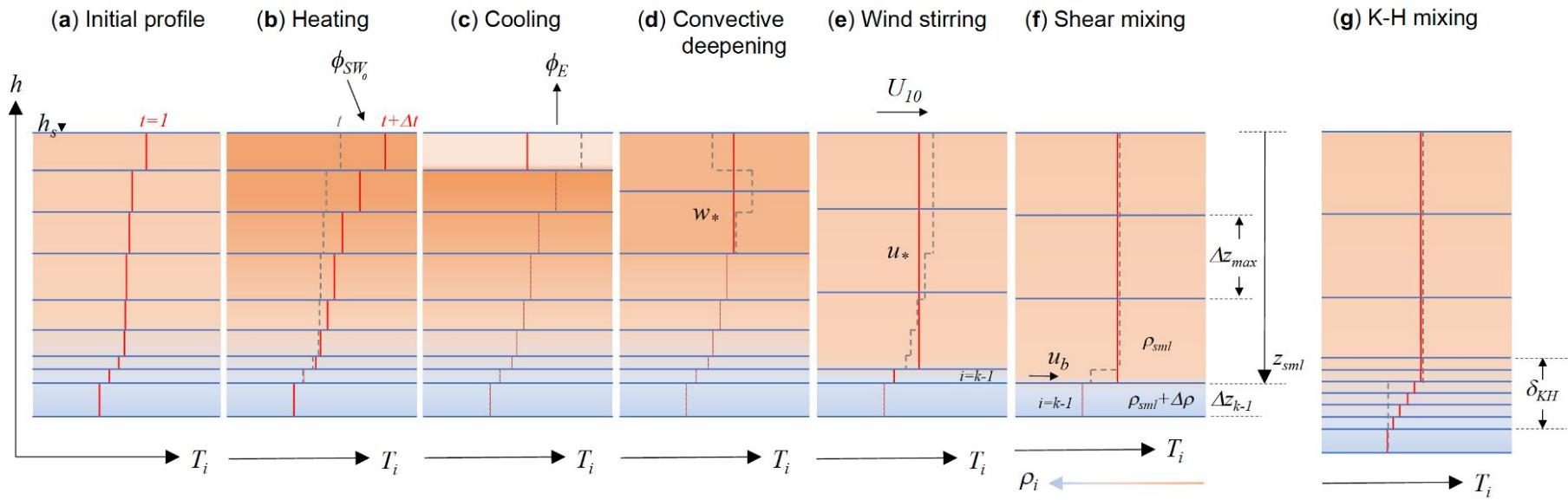


# Mixing I

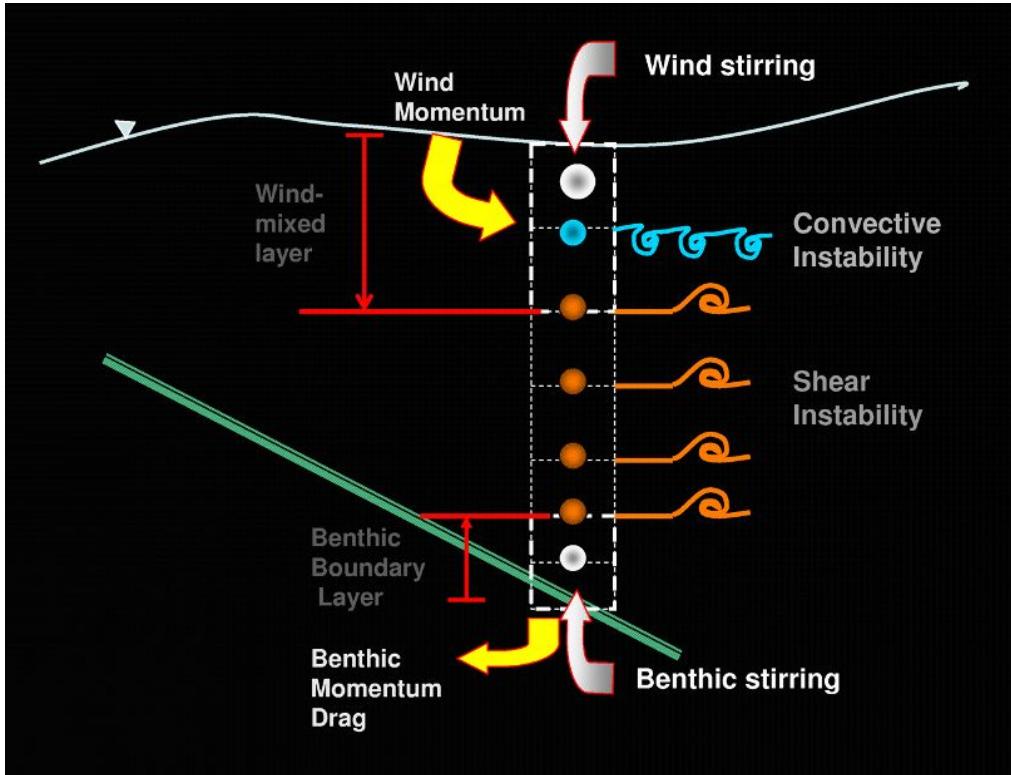
- Surface layer: energy balance approach
  - Energy balance determines thickness of surface mixed layer
  - Below surface mixed layer, turbulent diffusion approach is used
- Here, mixing depends on difference between potential energy and available kinetic energy
- Kinetic energy = convective overturn,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



# Mixing II



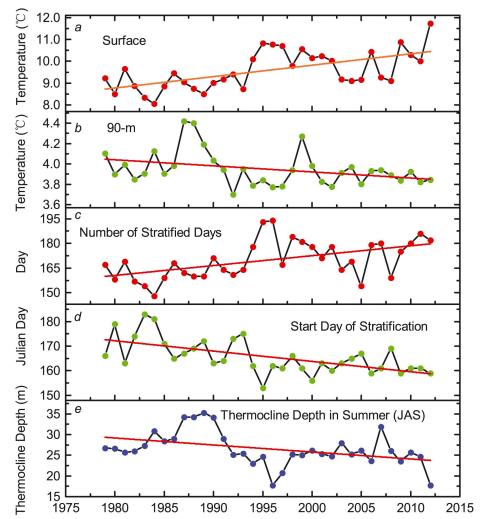
# Mixing III



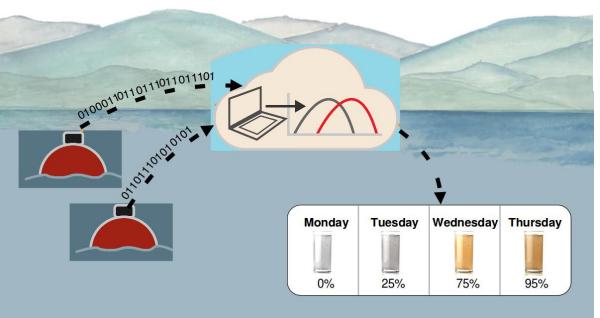
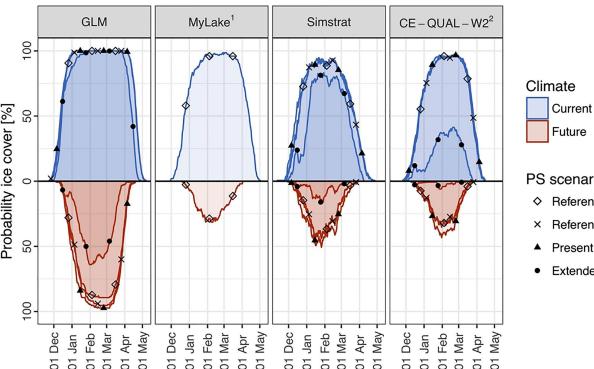
Kelvin-Helmholtz instabilities

# Example applications

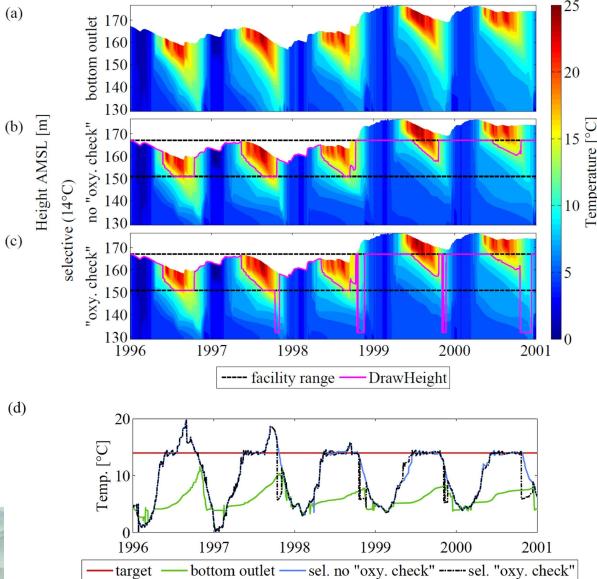
## Climate change effects on lakes<sup>1</sup>



## Future ice cover shifts<sup>2</sup>



## Optimal withdrawal depth in reservoirs<sup>4</sup>



## Smart ecological forecasting (FLARE)<sup>3</sup>

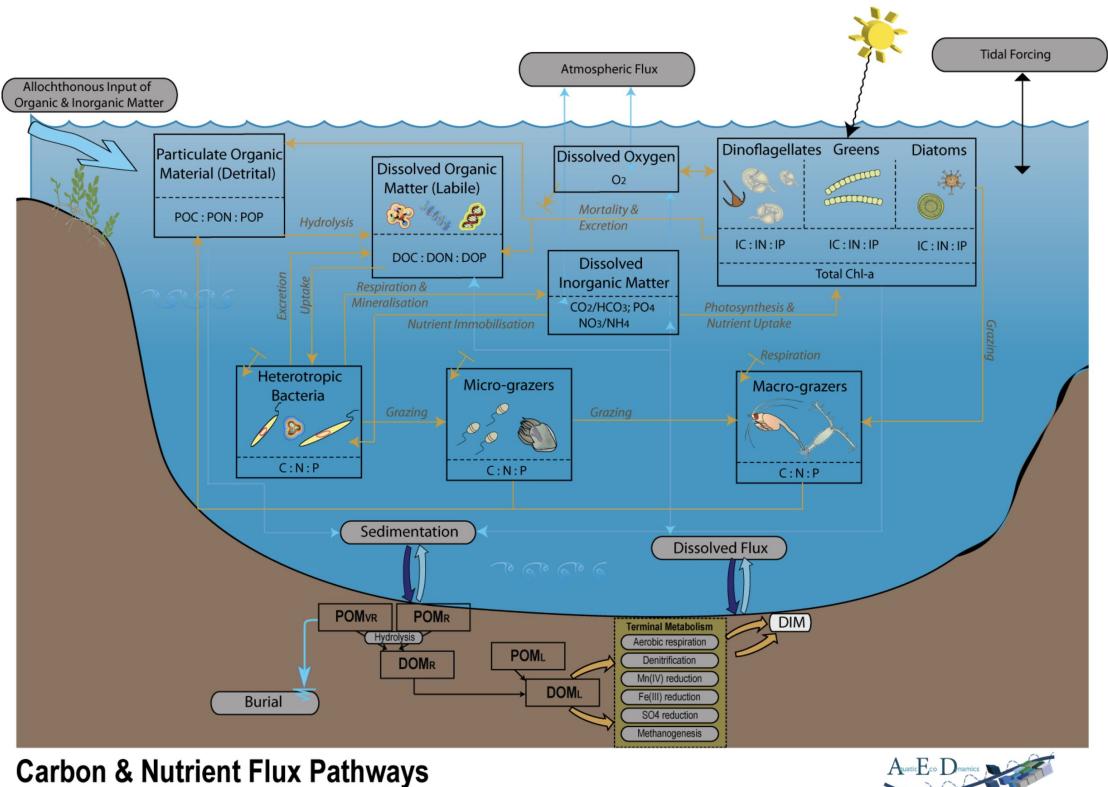
<sup>1</sup>Huang et al. 2017; <sup>2</sup>Kobler et al. 2019; <sup>3</sup>Figueiredo, Thomas, Carey & Weathers; <sup>4</sup>Weber et al. 2017

# AED2

# theory

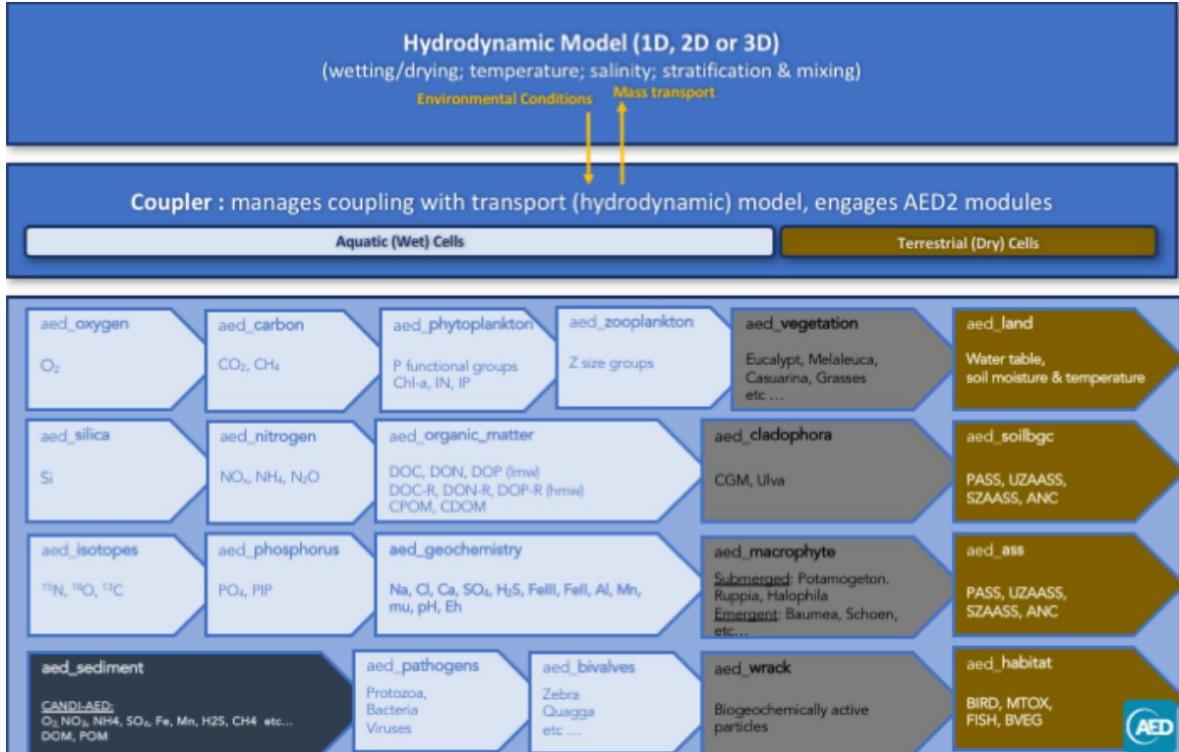
# AED2: water quality model

- Conceptualize your individual ecosystem:
  - Oxygen, nutrients, phytoplankton
  - Sediment biogeochemistry
  - Benthic communities
- Interacts with GLM (two-way coupling)



# AED2: modularised structure

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

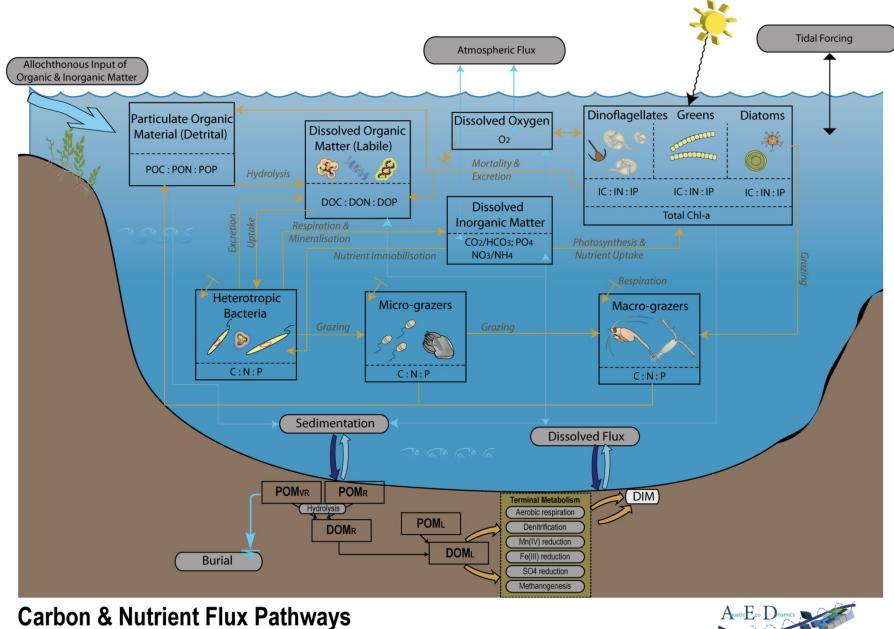


# AED2: dissolved oxygen

atmospheric exchange sediment oxygen demand

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

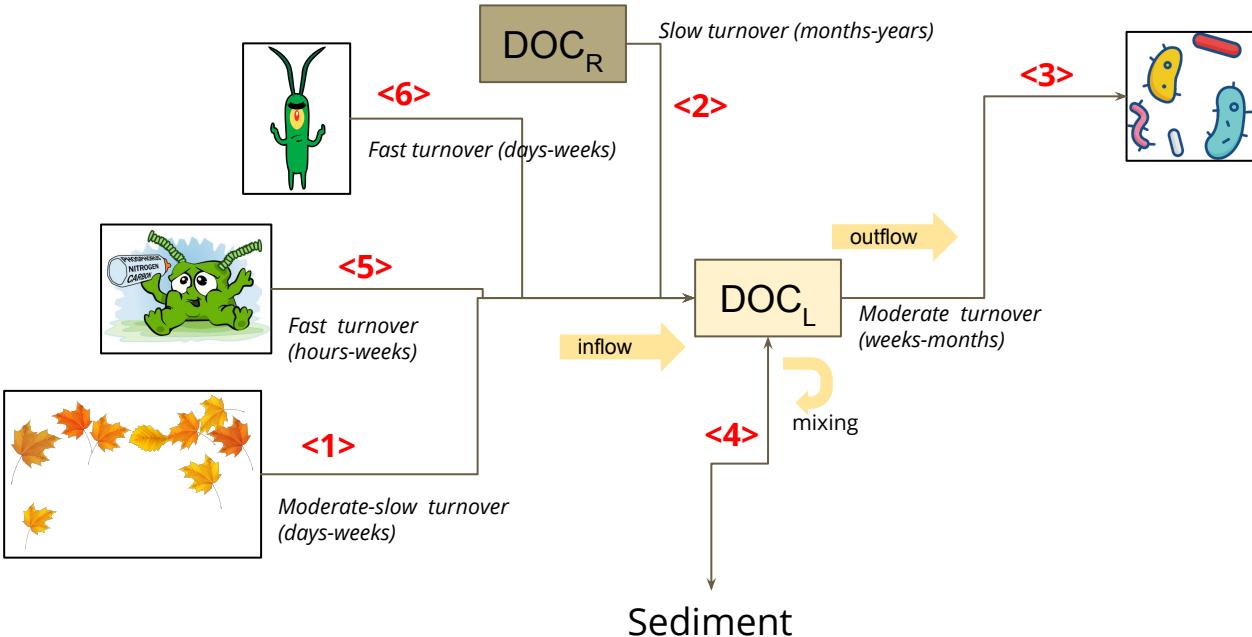
- Fast moving pool (minutes to days)
- Solved over vertical axis
- Plus advection and diffusion
- Photosynthesis/respiration = phytoplankton, zooplankton, seagrass, bivalves



# AED2: dissolved organic carbon - concept

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

<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: 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

$$\frac{dPOC}{dt} = f_{bdown}^{CPOM} - f_{decom}^{POC} - f_{sett}^{POC} + \sum_a^{N_{PHY}} f_{mort}^{PHY,C_i} + \sum_z^{N_{ZOO}} [(1 - k_{assim}^z)f_{assim}^z + (1 - k_{fse}^z)f_{fse}^z + f_{mort}^z]$$

- = + 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 DOM

$f(O_2)$  = scales from 0-1 based on  $[O_2]$

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

$$f_{miner}^{VAR} = R_{miner}^{VAR} \frac{[O_2]}{K_{miner} + [O_2]} (\theta_{miner})^{T-20} [VAR] \quad (15)$$

$$+ f_{denit}^{NO_3} \chi_{denit}^{VAR} \quad (16)$$

Anaerobic mineralization of DOM

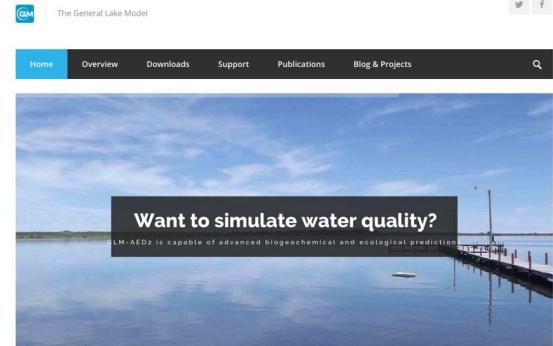


RDOC, minimum-maximum rate of aerobic mineralization of labile DOC @20C ( $0.01\text{-}0.10\text{ d}^{-1}$ )

# Running GLM (in R)

# Setting up GLM

- Installing GLM:
  - Download software package via AED GLM website:  
[http://aed.see.uwa.edu.au/research/models/GLM/latest\\_release.html](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")`)



The screenshot shows the GLM website's 'Downloads' page. At the top, there's a navigation bar with links for Home, Overview, Downloads, Support, Publications, and Blog & Projects. Below the navigation is a large image of a lake under a blue sky. A black banner across the image contains the text 'Want to simulate water quality? GLM-AED2 is capable of advanced biogeochemical and ecological prediction'. To the left of the banner is a small screenshot of a Mac OS X desktop showing a window titled 'Robert Ladwig / ...' with icons for Docker and Spring.

Below the banner, there are four circular sections with icons and text:

- Science Basis**: GLM is a 1-dimensional lake water balance and stratification model. It is distributed coupled with a powerful ecological modeling library to also support simulations of lake water quality and ecosystems processes.
- Suitability**: GLM is suitable for a wide range of natural and engineered lakes, from very shallow (e.g., mixed) and deep (stratified) systems. The model has been successfully applied to systems from the scale of individual ponds and wetlands to the scale of Great Lakes.
- Open Access**: GLM is an open-source project, and the source code is accessible and customizable for specific applications.

Below these sections is another navigation bar with links for Home, Overview, Downloads (which is highlighted in blue), Support, Publications, and Blog & Projects.

The main content area features a section titled 'Latest Release' with a horizontal line. Below it is a section for 'GLM V3.0 (2019 release)' with two buttons: 'Download Model' (blue background) and 'Source Code'. There's also a 'Notes:' section with two bullet points:

- ✓ GLM: The above GLM binary comes packaged with FABM & AED2.
- ✓ GLM+: Note the GLM+ version is GLM coupled with AED2 & AED2+. This is made available on request.

# 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

```
1 !-----  
2 ! general model setup  
3 !-----  
4 &glm_setup  
5   sim_name = 'Mendota'  
6   max_layers = 75  
7   min_layer_vol = 0.1  
8   min_layer_thick = 0.15  
9   max_layer_thick = 1.5  
10  density_model = 1  
11 /  
12 &mixing  
13   surface_mixing = 1  
14   coef_mix_conv = 0.2  
15   coef_wind_stir = 0.23  
16   coef_mix_shear = 0.3  
17   coef_mix_turb = 0.51  
18   coef_mix_KH = 0.3  
19   coef_mix_hyp = 0.4689587  
20   deep_mixing = 2  
21   diff = 0  
22 /  
23 &light  
24   light_mode = 0  
25   n_bands = 4  
26   light_extc = 1, 0.5, 2, 4  
27   energy_frac = 0.51, 0.45, 0.035, 0.005  
28   Benthic_Imin = 10  
29   Kw = 0.4315141  
30 /  
31 !-----  
32 ! water quality setup  
33 ! if this block is read, water quality functionality will be enabled  
34 !-----
```

# 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

# Setting up GLM

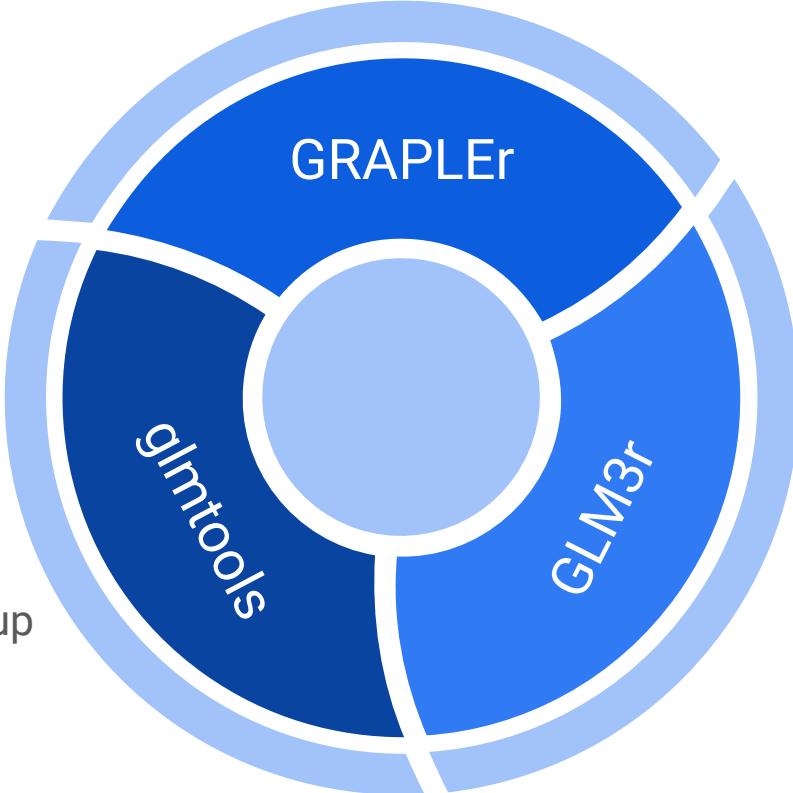
- Boundary conditions: data that drive the model
- At minimum, GLM needs meteorological data (hourly or daily) in CSV-format

```
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 in R

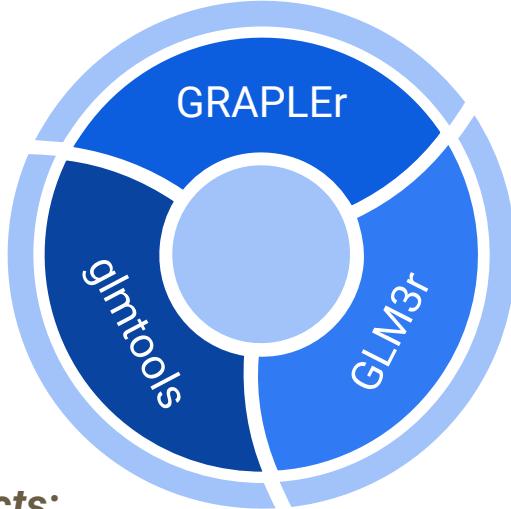


- Changing model setup
- Visualizing results
- Physical derivatives
- Calibration

- Distributed computing system
- Run multiple GLM simulations

- Run GLM in R

# GLM in R



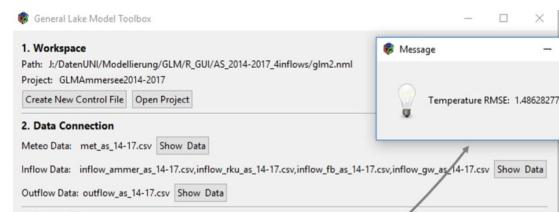
*More awesome R-related GLM projects:*

[Macrosystems EDDIE](#): classroom modules to teach macrosystems ecology

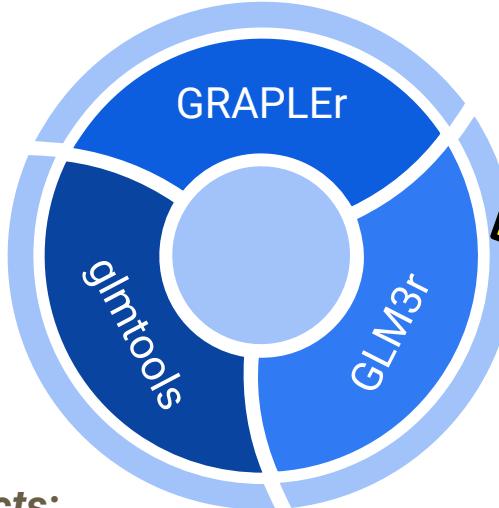
[LakeEnsemblR](#): R-package to run lake ensembles (release soon)

[glmGUI](#): GUI and toolbox to run GLM

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



# GLM in R



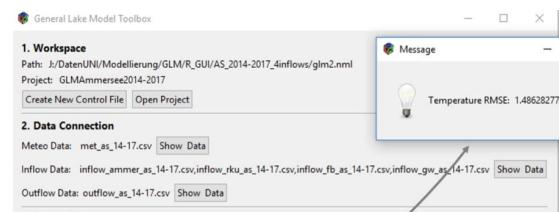
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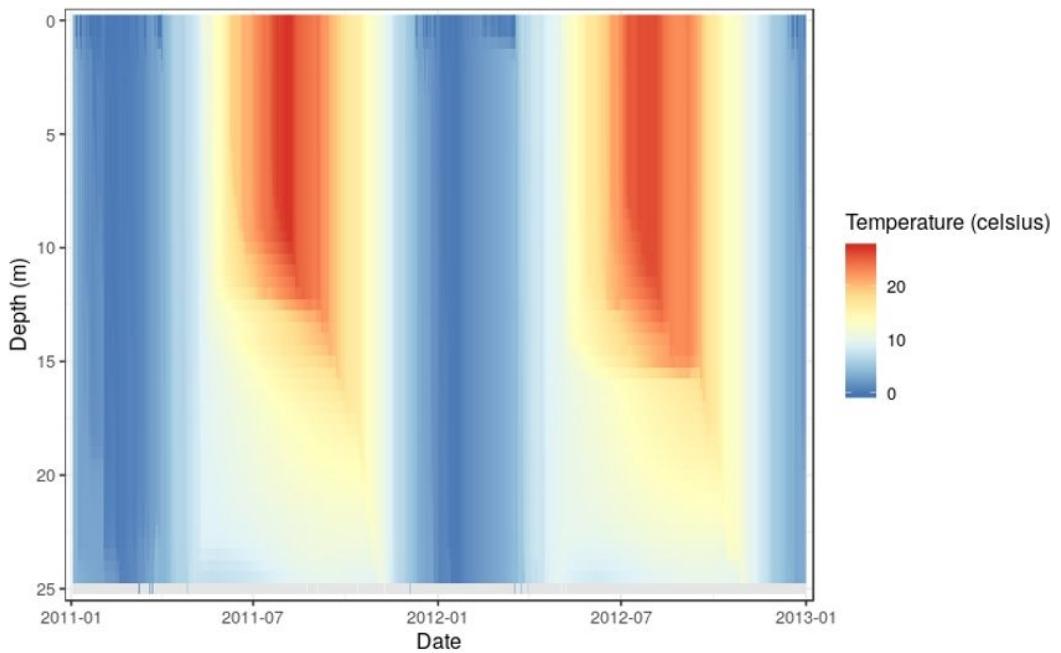
[glmGUI](#): GUI and toolbox to run GLM

[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)



# Finally some



# Wrapping up

Questions, issues, problems & feedback?

Join the official GLM slack



Thanks for joining!

Have fun lake modeling!



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@hydrobert