



WISCONSIN
UNIVERSITY OF WISCONSIN-MADISON



Introduction to running, visualizing, and calibrating the General Lake Model

Hilary Dugan, Robert Ladwig, Paul Hanson

GLEON 21



THE UNIVERSITY OF
WESTERN
AUSTRALIA

UF
UNIVERSITY of
FLORIDA

Find all material and data here

https://github.com/gsagleon/G21_GSA_workshop/tree/master/D_GLM

Who some of us are



Hilary Dugan
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Univ. of Florida



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UW-Madison

We're around all week, so feel
free to ask questions and engage
on the GLM Slack channel →



Some acknowledgements

GLM was developed by Matt Hipsey, Louise Bruce, Casper Boon; further contributions by Brendan Busch, Jordi Prats, Quinn Thomas, Wentao Guo, Cayelan Carey

GLM3r: Jordan Read, Luke Winslow, Joseph Stachelek, Laura DeCicco, Hilary Dugan, Robert Ladwig

glmtools: Jordan Read, Luke Winslow, Jordan Stachelek, Stuart Jones, David Watkins, Hilary Dugan, Robert Ladwig, Tadhg Moore

GRAPLER: Kensworth Subratie, Saumitra Aditya, Renato Figueiredo, Cayelan Carey, Paul Hanson

We probably missed some people. Sorry.

Scope of this workshop

- **At the end, you'll be able to run, visualize and calibrate a lake model using Rstudio**
- On the way:
 - Introduction to numerical modeling
 - How does GLM work?
 - Glimpse of how the water quality model works
 - Which packages are available in R?
 - What are the plans for the future?
 - How can I contribute to the development?



Scope of this workshop

2-2:45

- Introduction to modeling and GLM
- Introduction to glmtools
- Running GLM in R

3-3:45

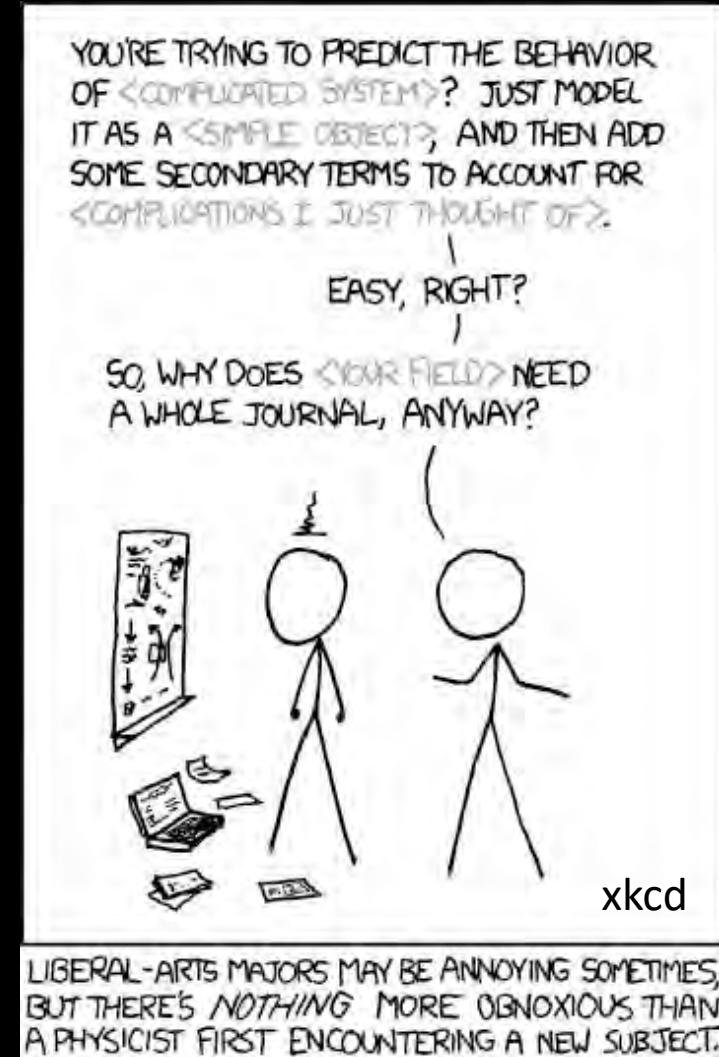
- Visualizing and calibrating GLM in R
- Introduction to GRAPLER

4-4:30

- Current and future developments
- Community involvement

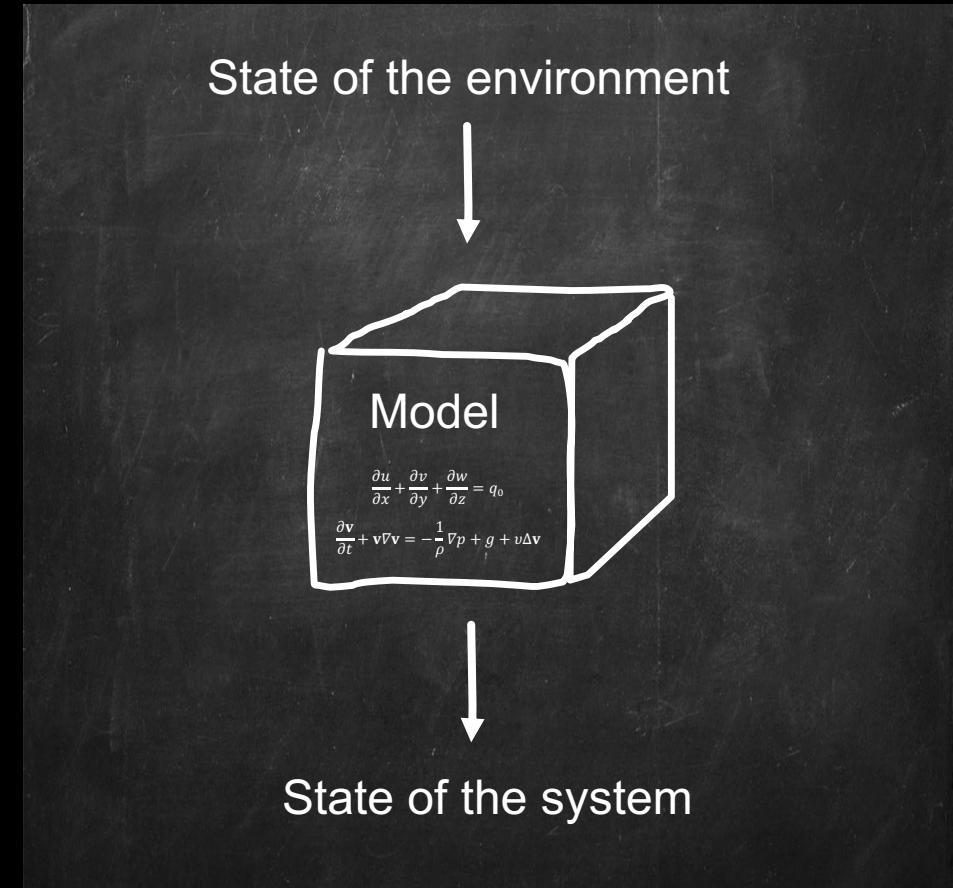
Crash course: Numerical Modeling

- 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)



Crash course: Numerical Modeling

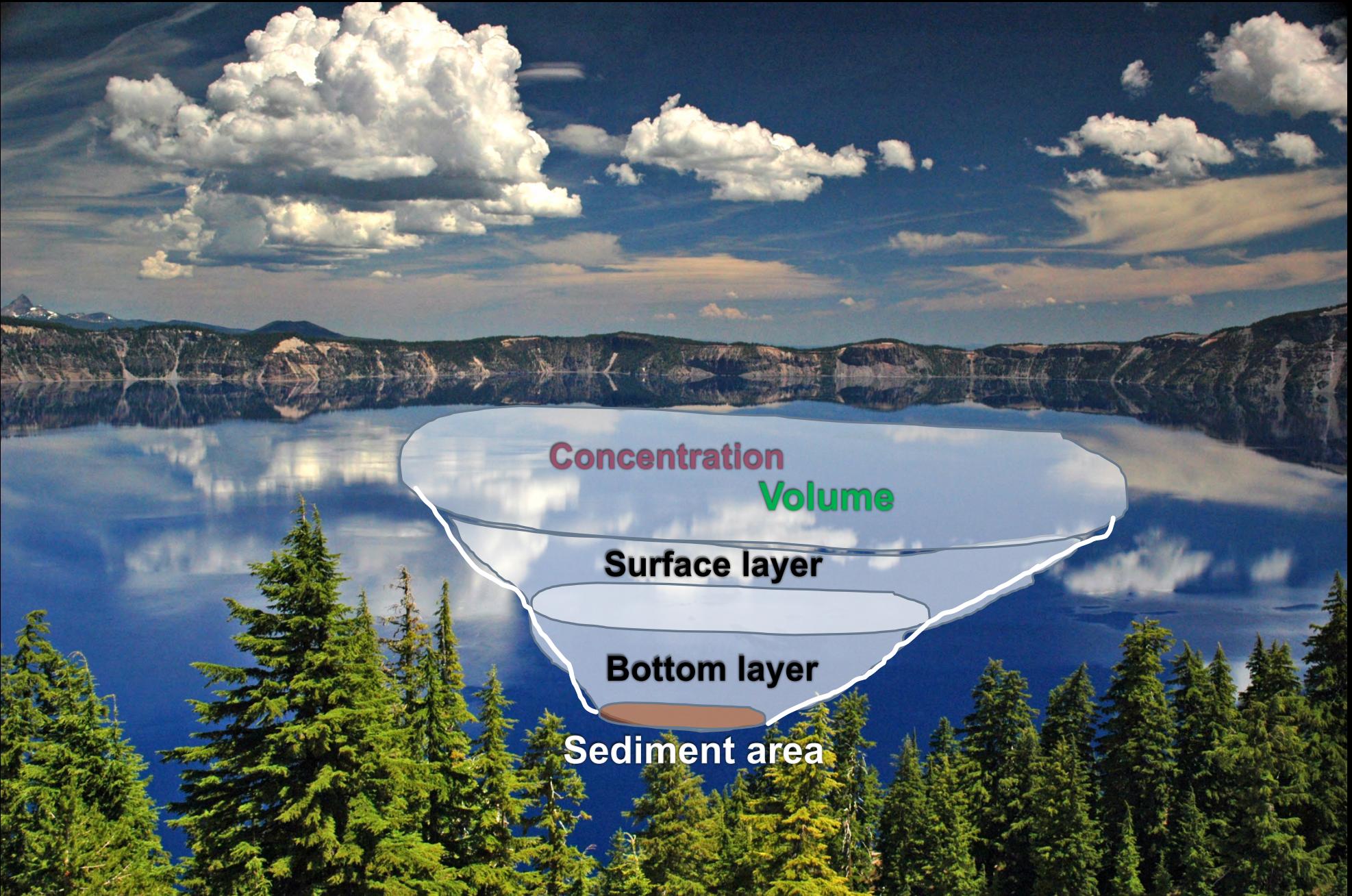
- **Conservation of mass (continuity)**
 - Inflow(s)= outflow(s)
 - Mass cannot be created or destroyed
- **Conservation of momentum**
 - Velocity based on balances of forces (gravity, pressure, friction, earth-rotation)



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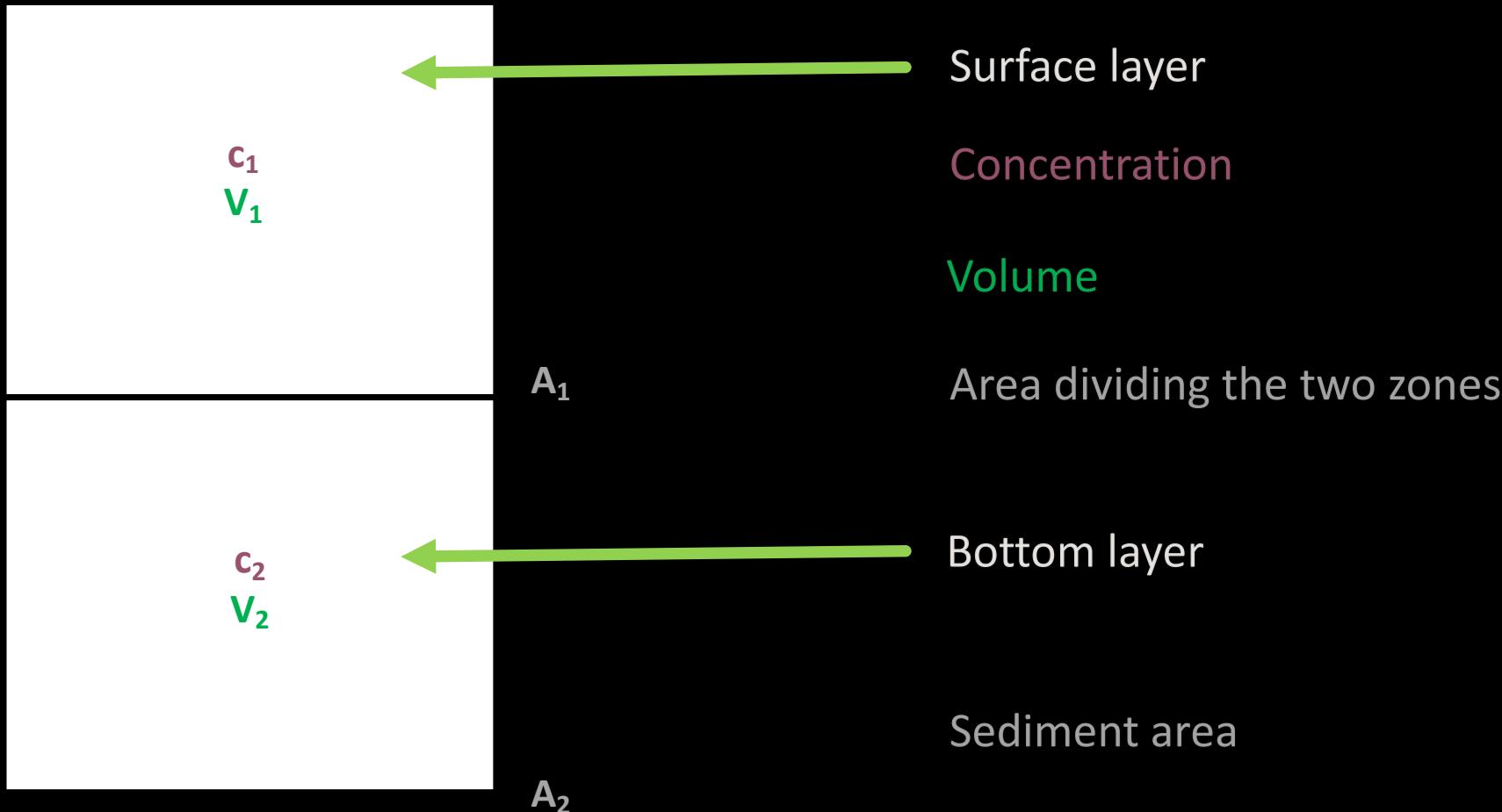


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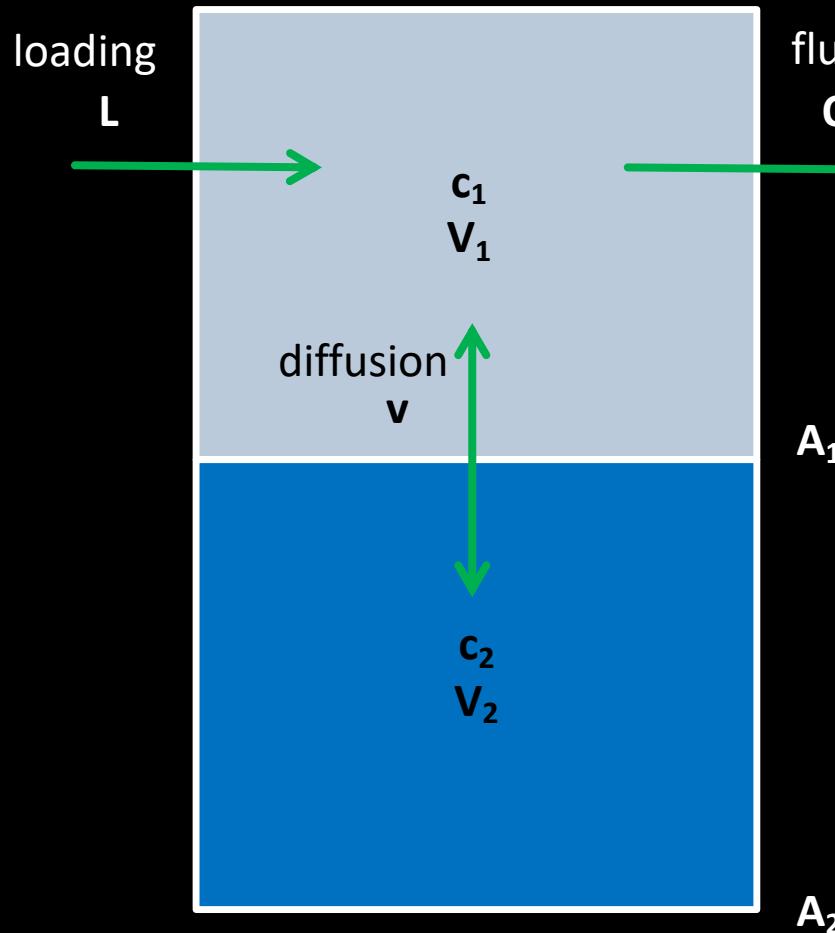
Crash course: Numerical Modeling

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



Crash course: Numerical Modeling

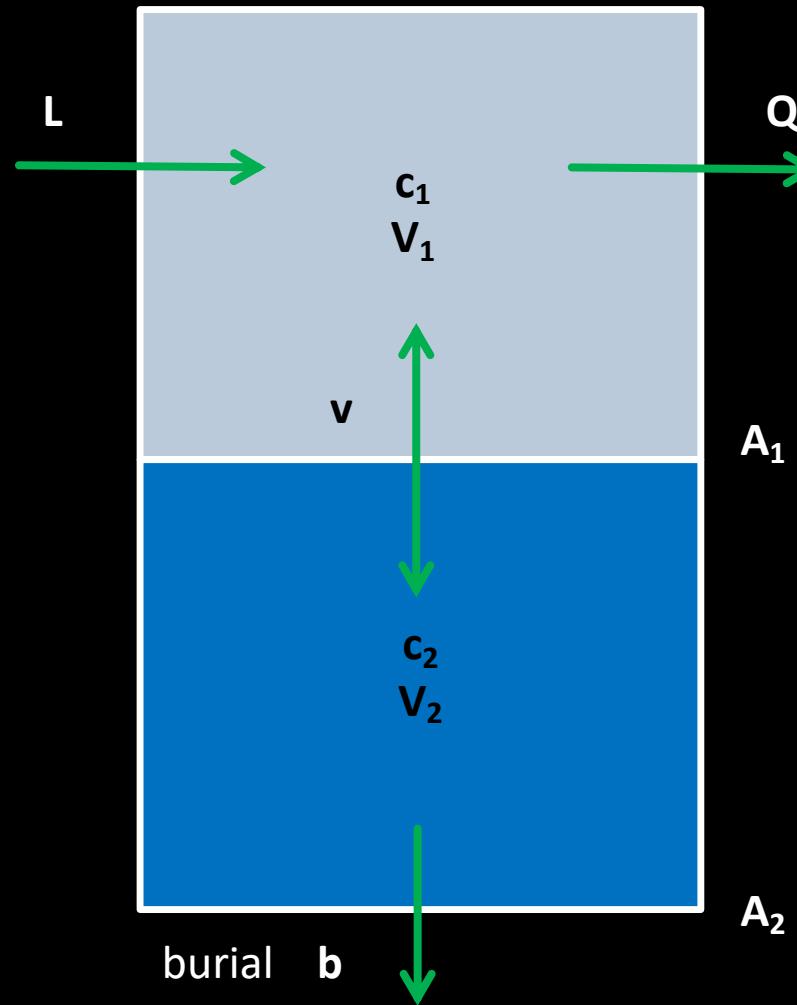
Most are bookkeeping exercises to keep inflow = outflow (mass-balance)



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

Crash course: Numerical Modeling

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

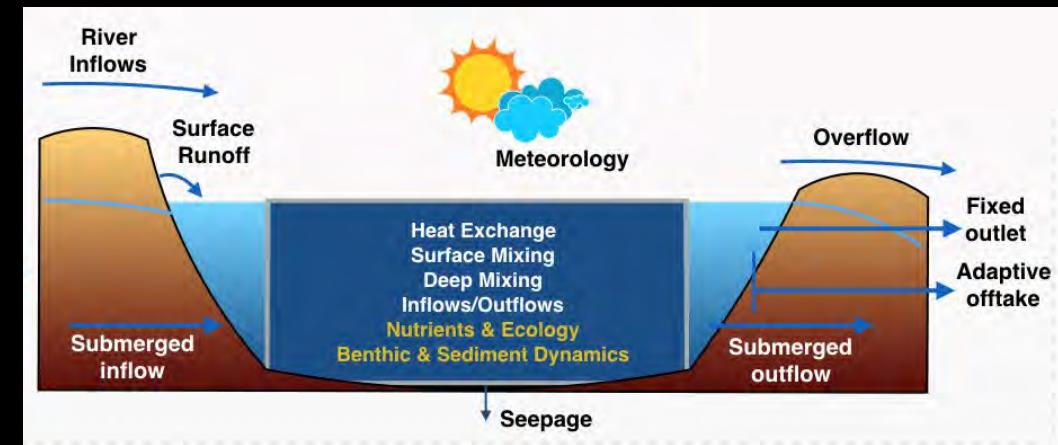


$$\frac{dc_1}{dt} = \frac{L - Qc_1 + vA_1(c_2 - c_1)}{V_1}$$

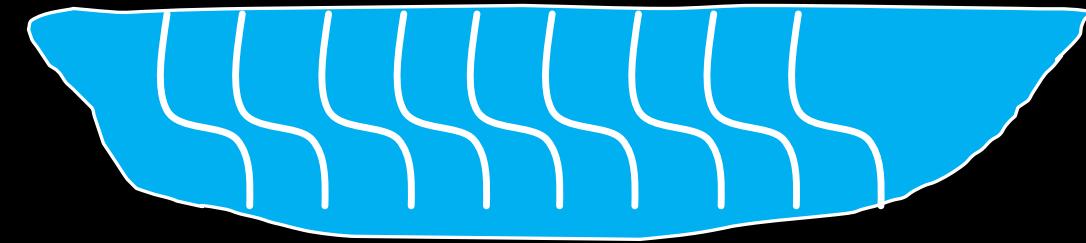
$$\frac{dc_2}{dt} = \frac{vA_1(c_1 - c_2) - bA_2c_2}{V_2}$$

Introduction to GLM

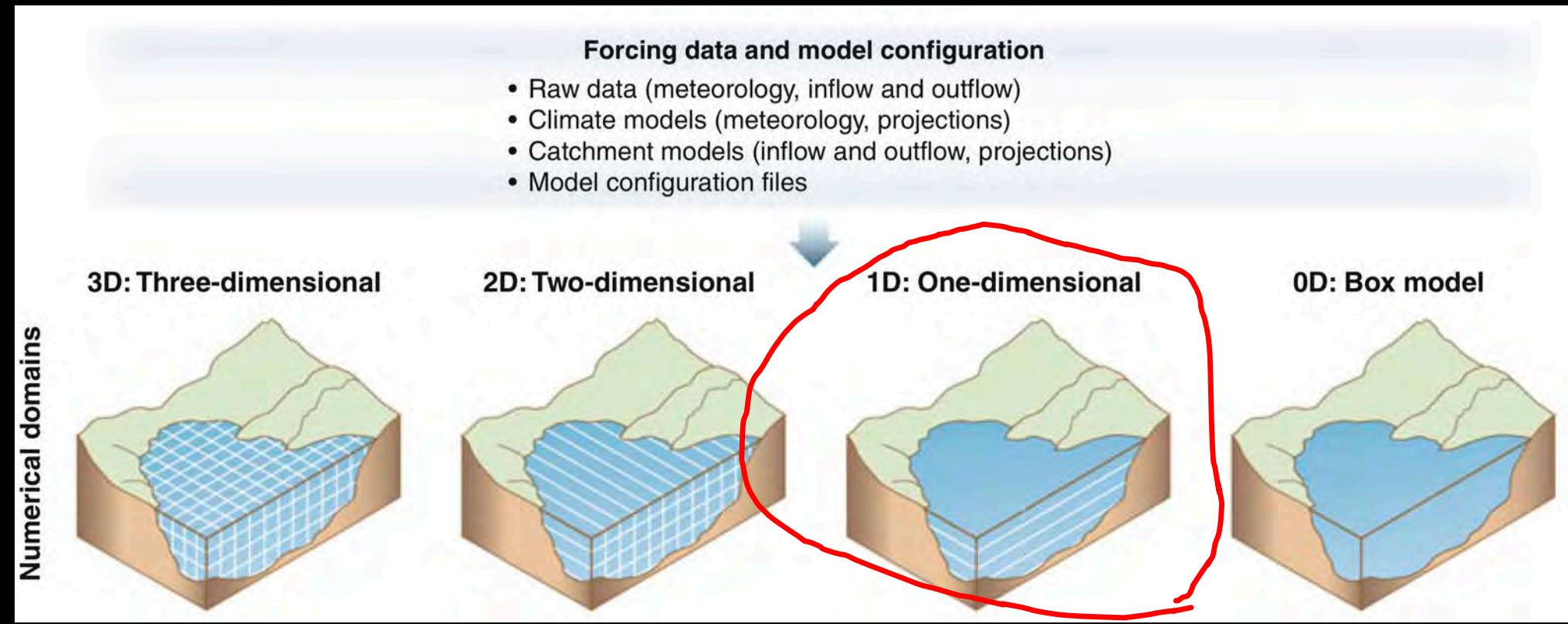
- Supported as a project within GLEON
- Developed by Matt Hipsey, Louise Bruce and Casper Boon at UWA
- Designed to operate with the Aquatic EcoDynamics Model Libraries (AED) → water quality model
- Languages: C (and Fortran for AED)
- Freely available as open-source program
- <https://github.com/AquaticEcoDynamics/GLM>



Introduction to GLM

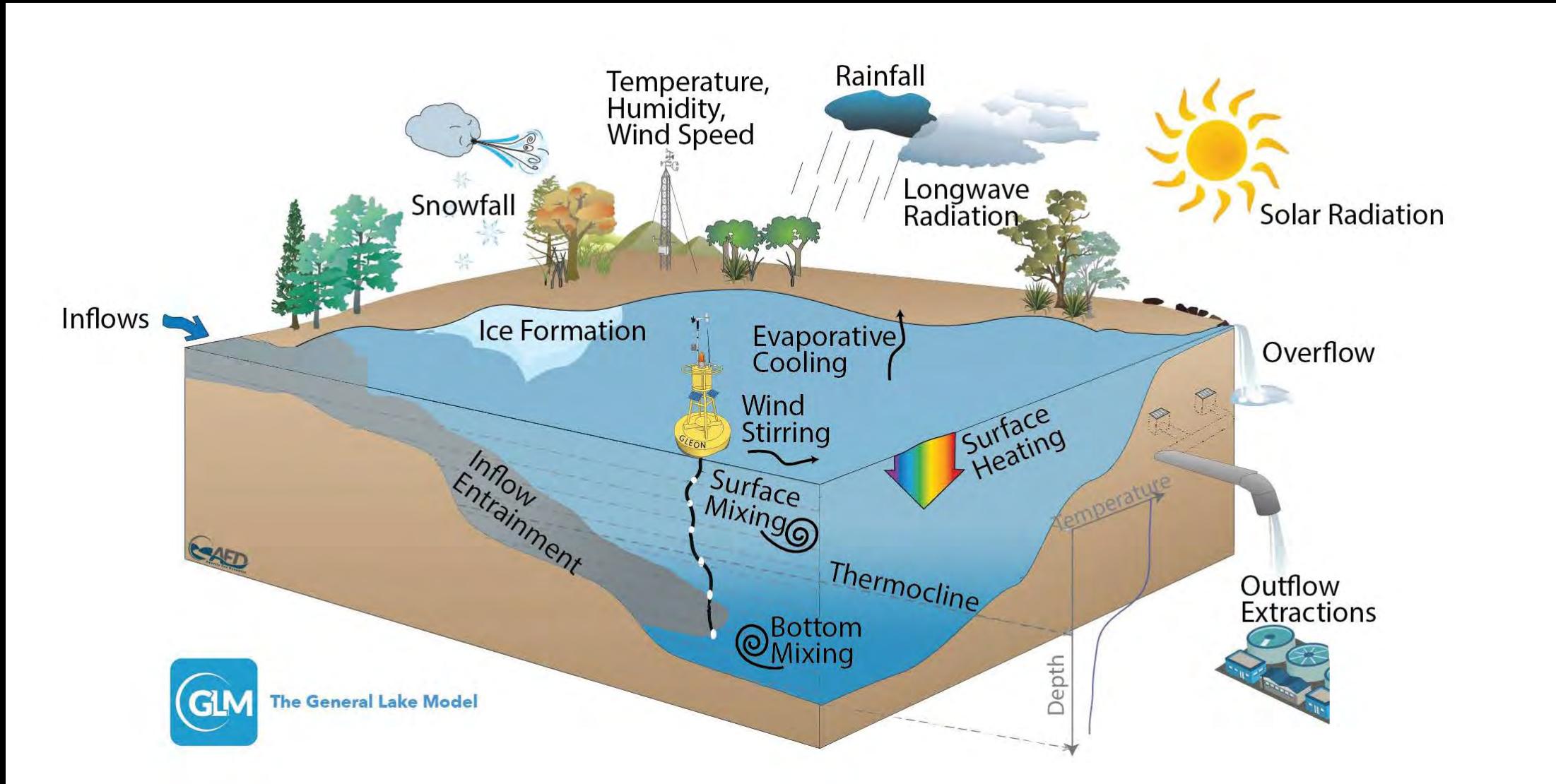


- Vertical one-dimensional model (spatially homogenous lake)



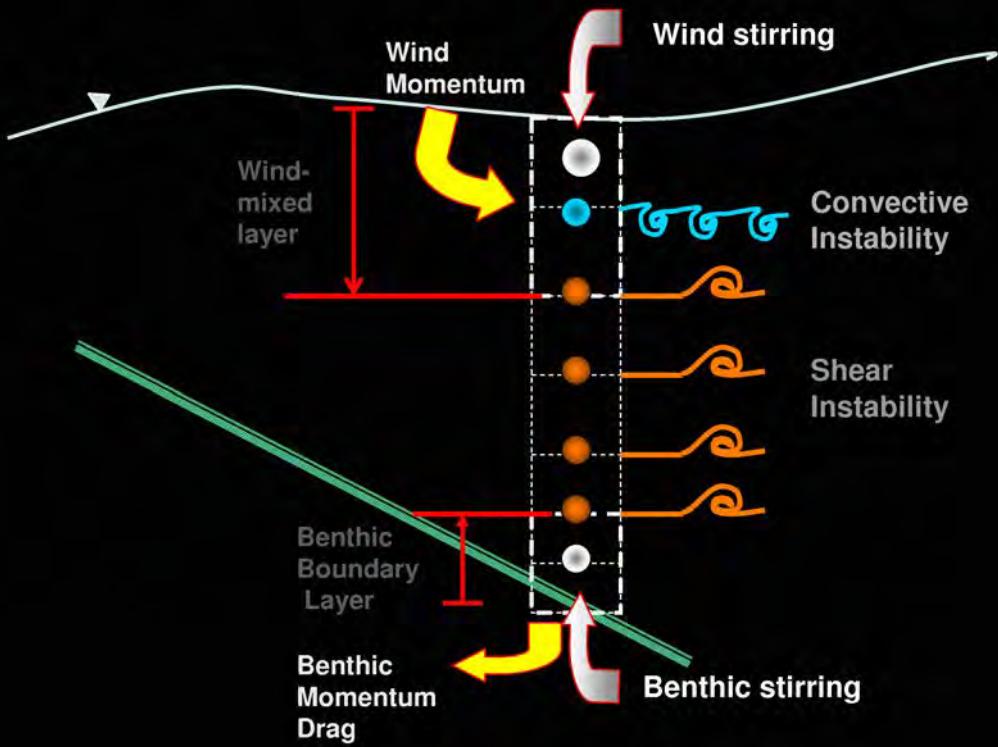
Trolle (2012)

Introduction to GLM

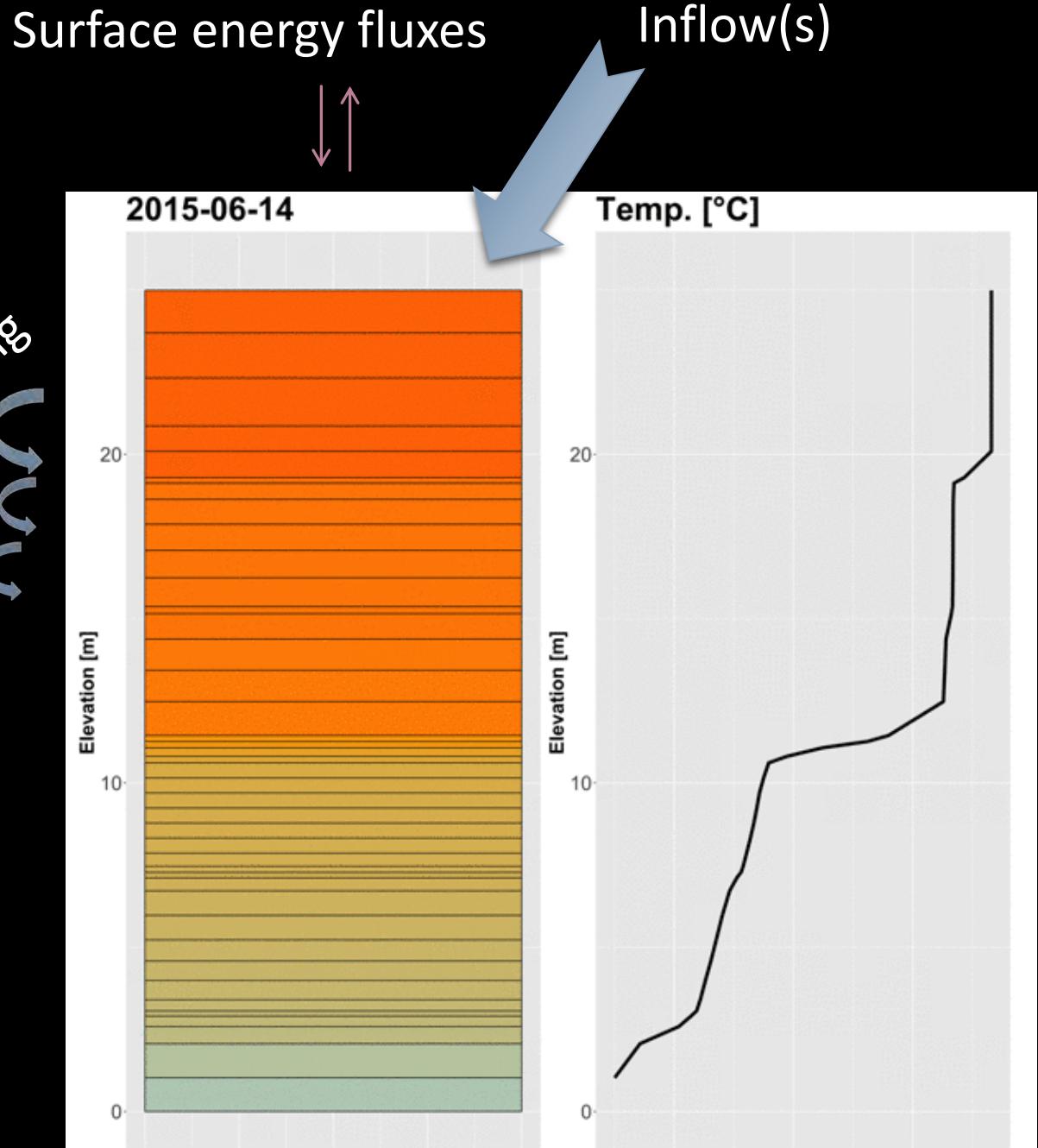


Introduction to GLM

- Flexible grid: thickness of layers
- Vertical mixing by stirring, convective overturn and shear



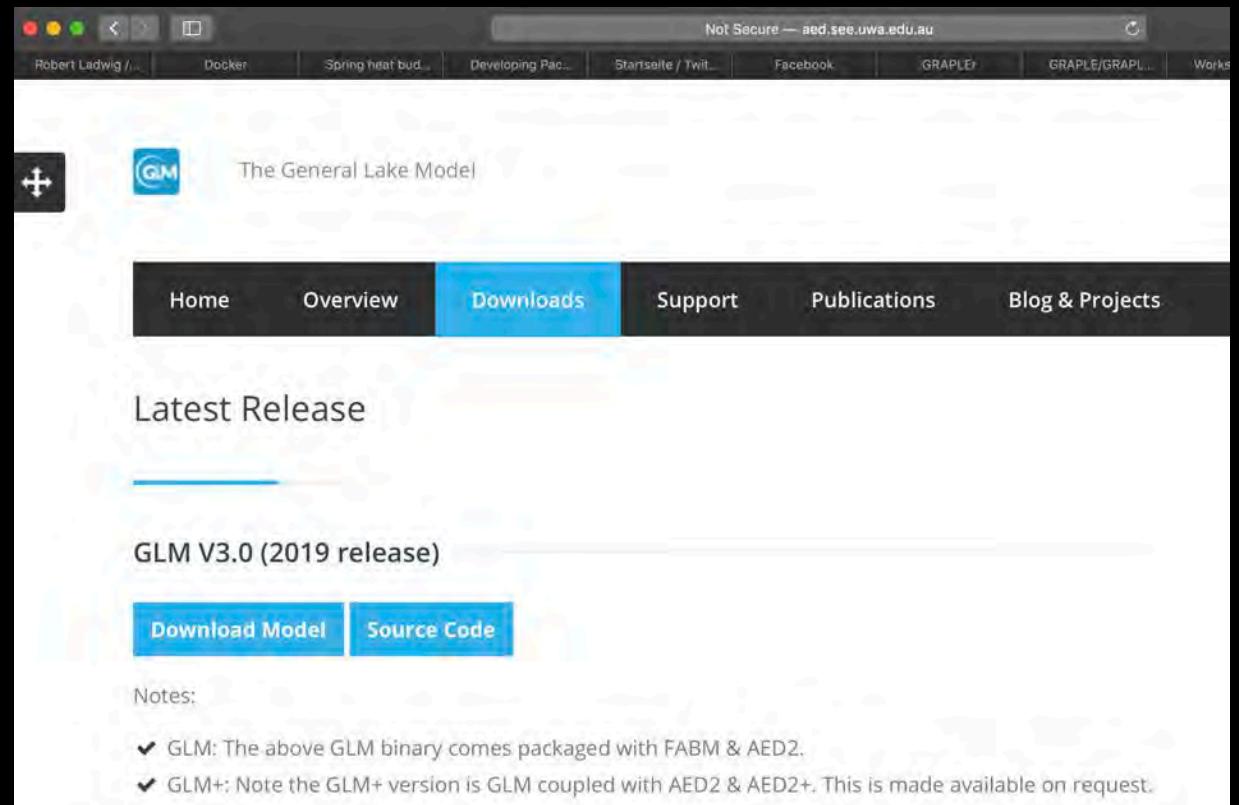
mixing ↗



Introduction to GLM

Installing GLM:

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



Introduction to GLM

- You've installed GLM (executables), what now?
- Main tool: *glm3.nml* 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  !-----
```

Introduction to GLM

- Main tool: `glm3.nml` file
- 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  
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30 /  
31 !-----  
32 ! water quality setup  
33 ! if this block is read, water quality functionality will be enabled  
34 !-----
```

Introduction to GLM : setting up your model

	glm3.nml file	
1. Define the morphometry	&glm_setup:	General simulation info
1. Area-depth relationship (hypsoigraphy)	&wq_setup:	Water quality
2. Define what you want to simulate	&time:	Time control
1. State variables (temperature, salinity, etc.)	&morphometry:	Lake morphometric information
2. Grid resolution and time step	&output:	Output file details
3. Define external environment	&init_profiles:	Initial vertical profiles
1. Boundary conditions (inflows, meteorology, outflows)	&meteorology:	Surface forcing and meeorology
4. Provide an initial condition	&inflows:	Information about inflowing rivers
5. Start your simulation	&outflows:	Information about outflows
	&light:	Information about light climate

Introduction to GLM : setting up your model

Model Configuration						
A GLM simulation is configured via the main "namelist" (nml) text file called <code>glm3.nml</code> . The key elements of this file are depicted as "blocks" in the above image and each block of configuration options & parameters is summarised in detail in the below table.						
&glm_setup	&mixing	&wq_setup	&morphometry	&time	&output	&init_profiles
&sediment	&snowice					
The first block IS compulsory, with the following variables that may be set :						
Variable Name	Symbol	Description	Type	Units	Options	Default
<code>sim_name</code>		Title of simulation	[string]			'lake'
<code>max_layers</code>	N_{MAX}	Maximum number of layers	[integer]	-		500
<code>min_layer_vol</code>	ΔV_{min}	Minimum layer volume	[real]	m^3		
<code>min_layer_thick</code>	Δz_{min}	Minimum thickness of a layer (m)	[real]	m		
<code>max_layer_thick</code>	Δz_{max}	Maximum thickness of a layer (m)	[real]	m		
<code>density_model</code>	Θ_ρ	Switch to set the density equation	[integer]	-	$\rho[T, S] \leftarrow \begin{cases} \text{TEOS-10: } & \Theta_\rho = 1 \\ \text{UNESCO(1981): } & \Theta_\rho = 2 \\ \text{custom: } & \Theta_\rho = 3+ \end{cases}$	1

GLM Online documentation
http://aed.see.uwa.edu.au/research/models/GLM/getting_started.html

- Describes variable names
- Gives units
- Shows options
- Provides a default value

Introduction to GLM

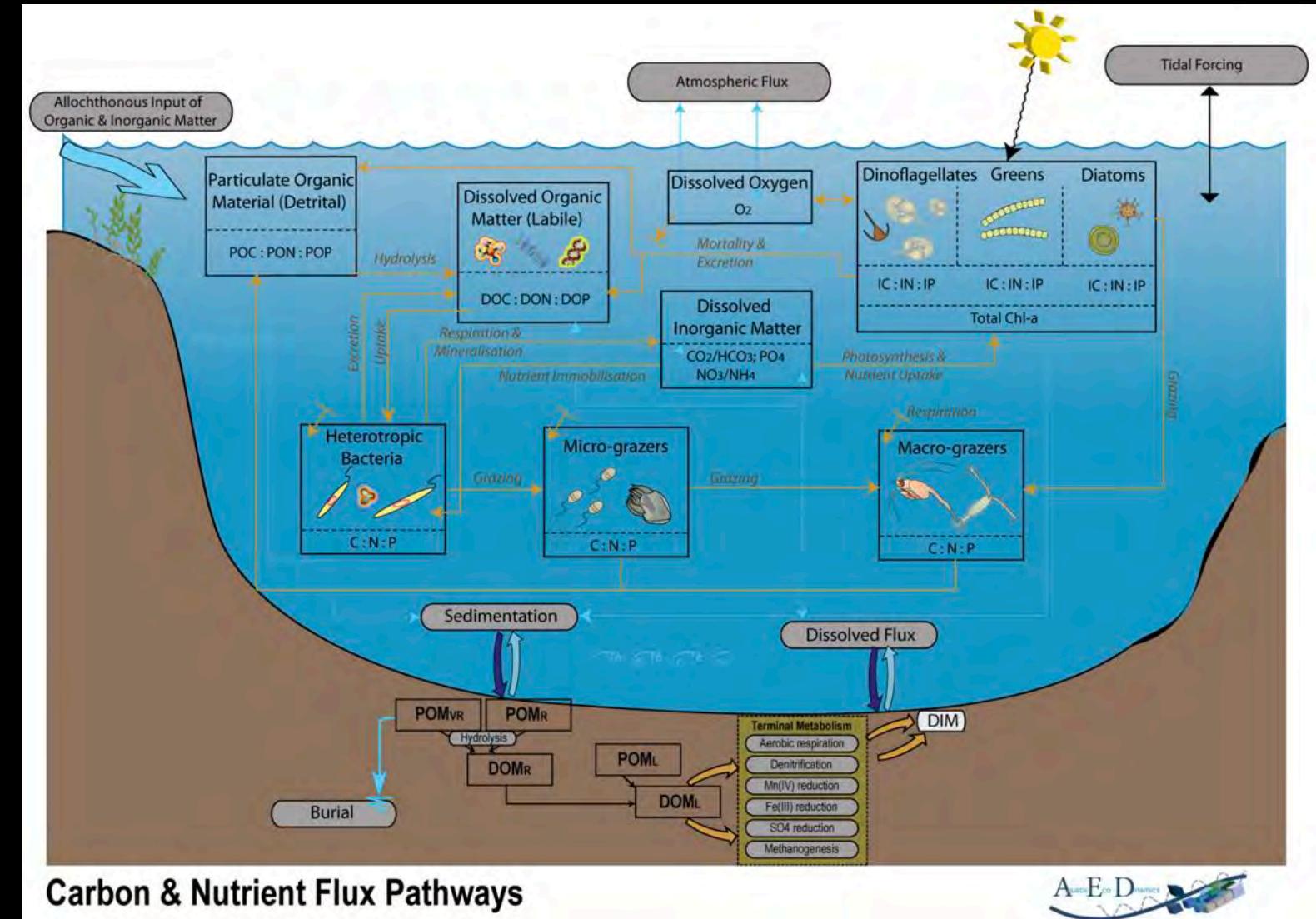
- Homepage:
<http://aed.see.uwa.edu.au/research/models/GLM/>
- Download newest versions of GLM
(currently v.3.0.5)
- Find support and help in Slack



The screenshot shows the official website for The General Lake Model. At the top, there's a navigation bar with links for Home, Overview, Downloads, Support, Publications, and Blog & Projects. The Home link is highlighted with a blue background. Below the navigation is a large banner image of a lake under a cloudy sky. Overlaid on the banner is a dark rectangular box containing the text "Want to simulate water quality? GLM-AEDz is capable of advanced biogeochemical and ecological prediction". To the left of the banner, there's a section titled "Science Basis" with a gear icon, describing GLM as a 1-dimensional lake water balance and stratification model. To the right, there are sections for "Suitability" (with a wrench icon) and "Open Access" (with a pen icon), both accompanied by detailed descriptions of the model's capabilities.

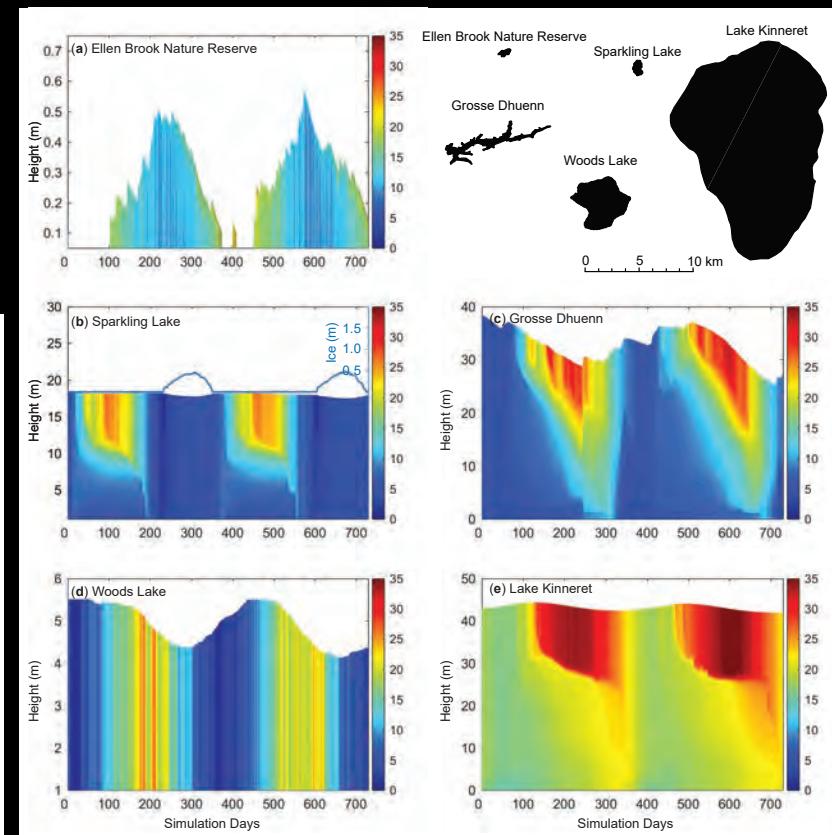
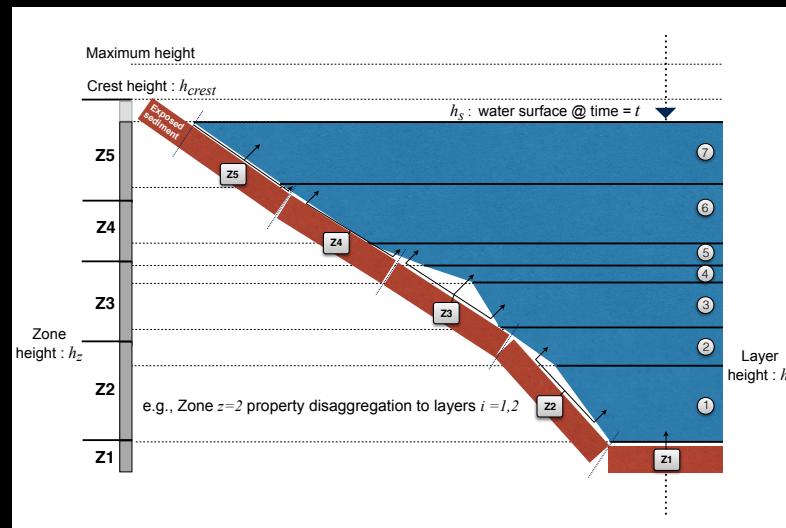
Sneak peek: Water Quality

- Aquatic Ecosystem Modelling Library (**AED2**)
- Consists of several modules to conceptualize individual ecosystems, eg:
 - oxygen, nitrogen, phosphorus, phytoplankton
 - sediment biogeochemistry
 - benthic communities
- GLM was designed to interact with AED2



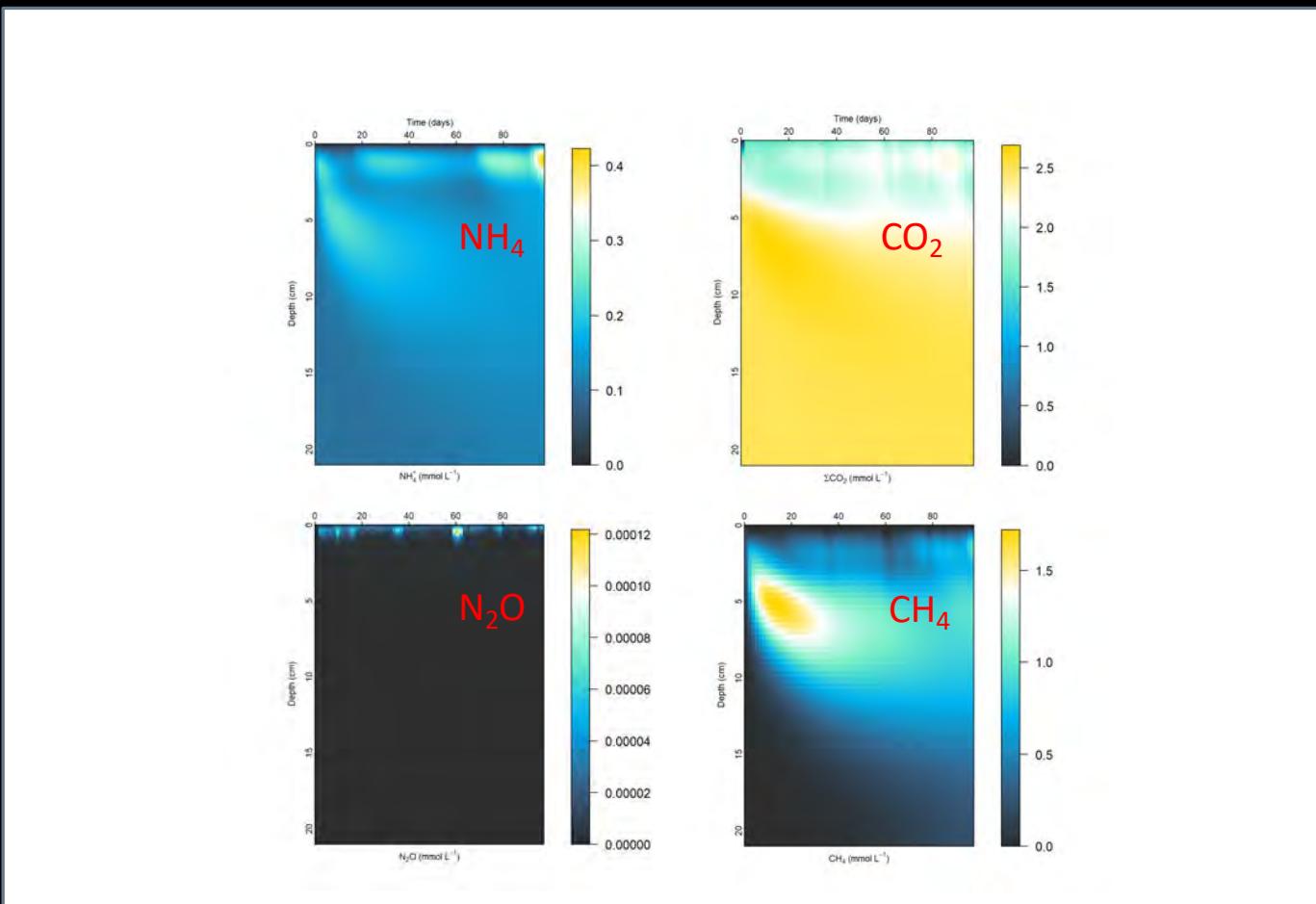
New features in v.3.X

- Sediment-depth zones and zone-specific sediment heating, and biogeochemistry
- Shallow lakes, ponds & wetland simulations (incl. drying out)
- Wind-sheltering options
- Seepage model
- Ice initialization
- Light model



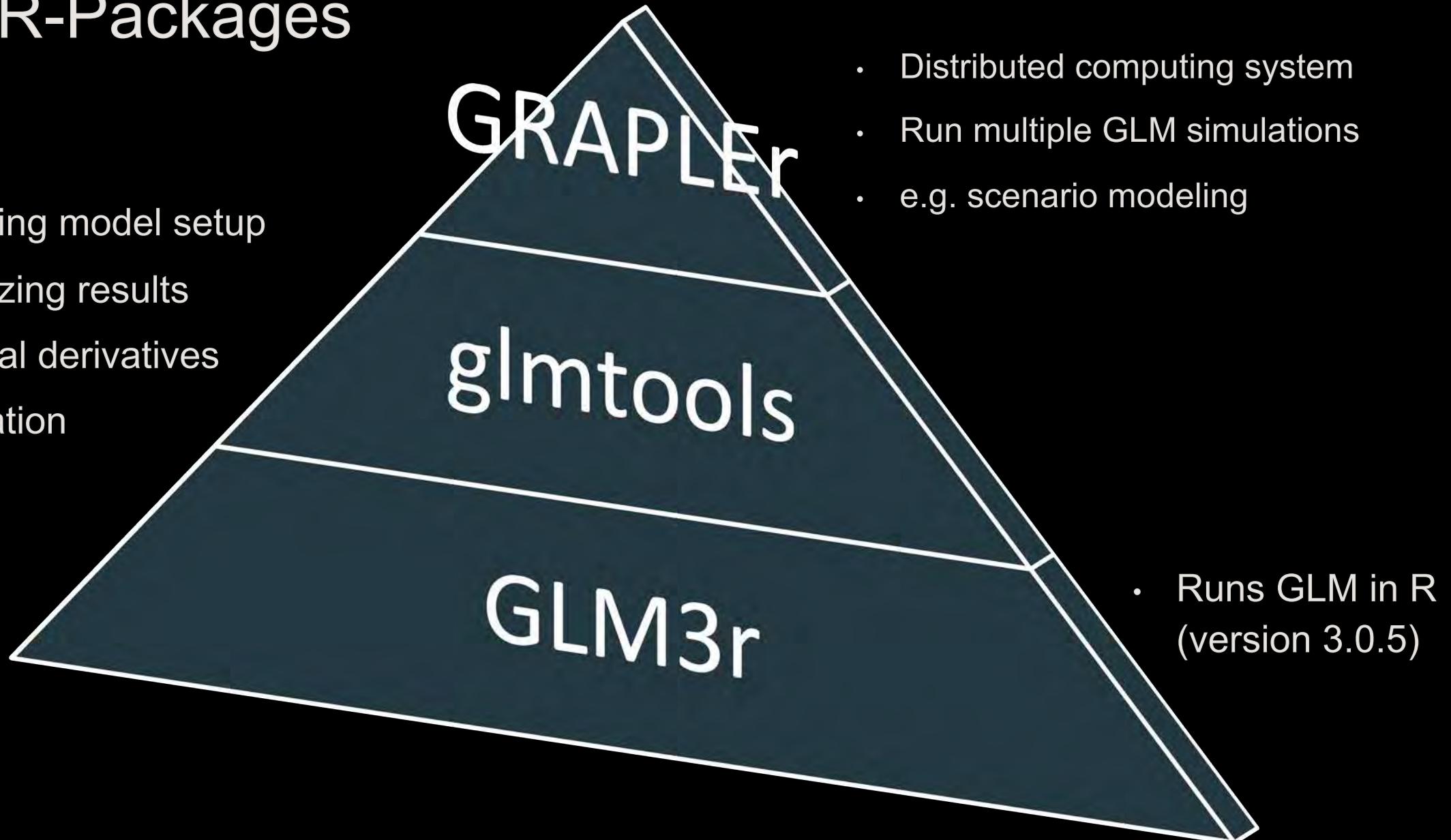
New features in v.3.X

- Water Quality updates (AED2 / AED2+) :
 - GHGs (N_2O , CH_4 , CO_2)
 - Benthic productivity (MPB, MAC, MAG)
 - Mussels (BIV)
 - Geochemistry (GEO)
 - Sediment diagenesis (SDG)



GLM R-Packages

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



GLM3r

- (big) Package that contains executables for Windows, Linux and macOS
- Current version: 3.0.5
- Runs GLM in R (with screen output)
- Also provides version number

Installation

You can install GLM3r from Github with:

```
# install.packages("devtools")
devtools::install_github("GLEON/GLM3r")
```

Usage

Run

```
library(GLM3r)

sim_folder <- system.file('extdata', package = 'GLM3r')

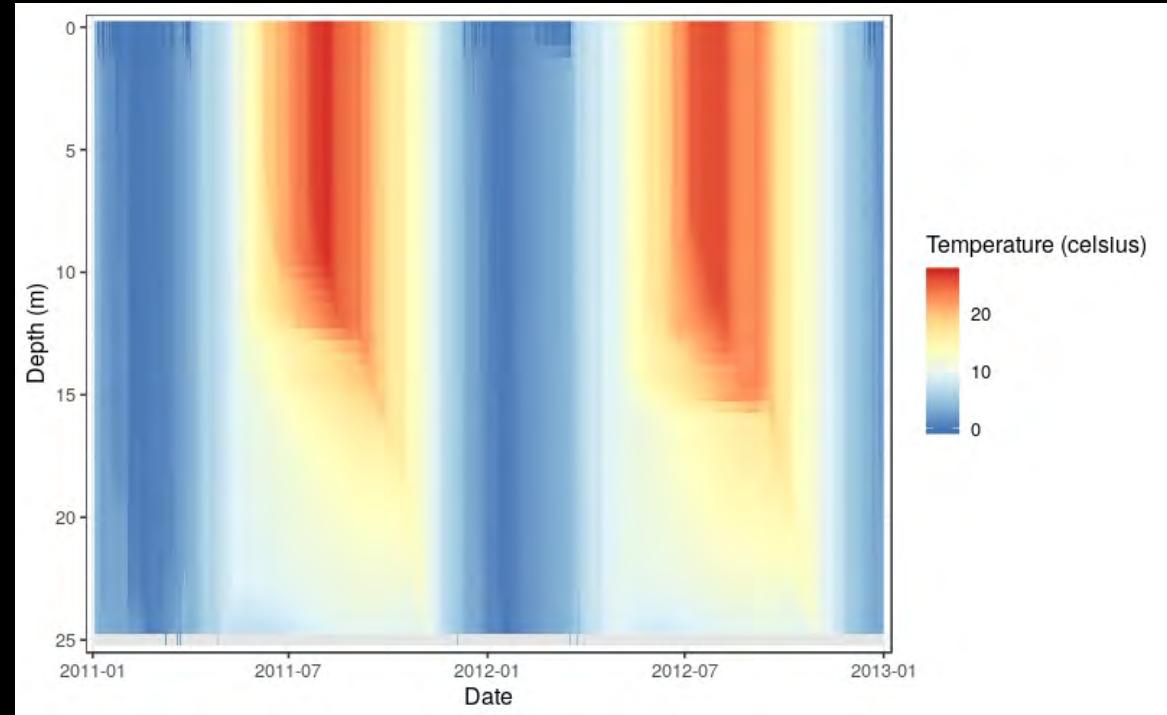
run_glm(sim_folder)
```

```
Reading config from glm3.nml
No WQ config
No diffuser data, setting default values
WARNING: Initial profiles problem - epected 0 wd_init_vals entries but got 30
-----
| General Lake Model (GLM) Version 3.0.5 |
-----
nDays 165825900 timestep 3600.000000
Maximum lake depth is 49.000000
Simulation begins...
Running day 2451636, 0.66% of days complete
Running day 2451637, 1.32% of days complete
---
Running day 2451785, 99.34% of days complete
Running day 2451786, 100.00% of days complete
Wall clock runtime 11 seconds : 00:00:11 [hh:mm:ss]
```

Run Complete

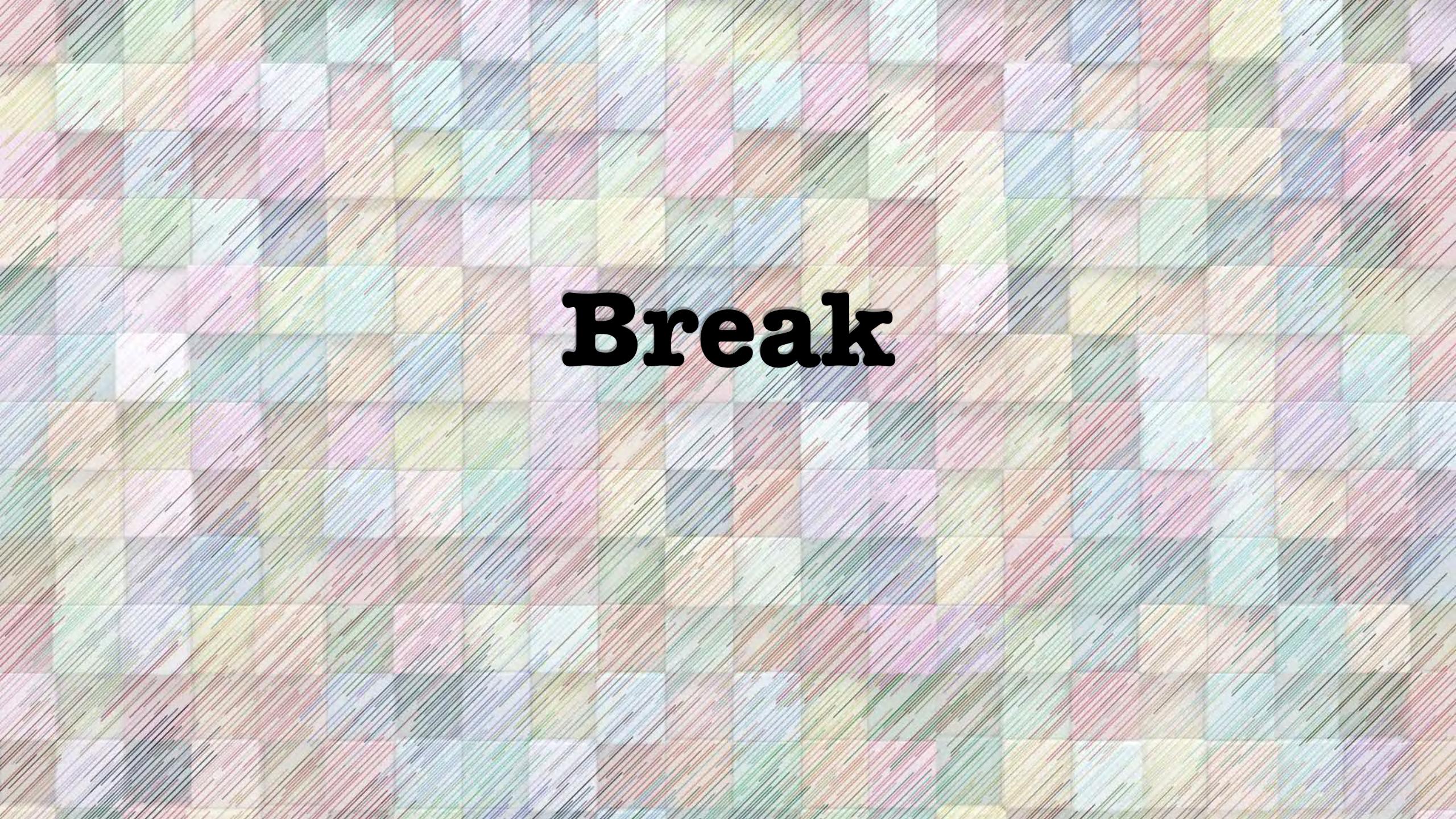
glmtools

- Either from github or from GRAN (USGS-R's alternative to CRAN)
- Offers **lots of functionalities**
 - Manipulate model setup
 - Retrieve data from output (evaporation, temperature data, ...)
 - Compare observed to simulated data
 - Visualize results (contour plots)
- New features:
 - **Overhauled visualization (ggplot2)**
 - Automatic **calibration**



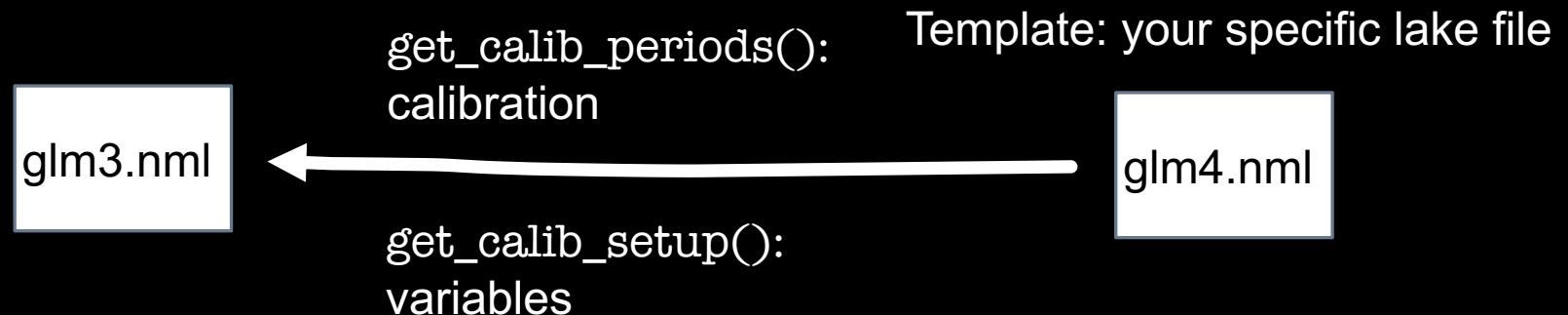
A scenic landscape featuring a calm lake in the foreground, framed by bare tree branches in the foreground. In the background, there's a dense forest and a sky filled with scattered clouds.

Run GLM in R



Break

glmtools: calibration



parameter	lower boundary	upper boundary	initial guess
-----------	----------------	----------------	---------------

	pars	lb	ub	x0
1	wind_factor	0.7	2.0	1.0
2	lw_factor	0.7	2.0	1.0
3	Kw	0.1	0.8	0.5
4	sed_temp_mean	3.0	8.0	5.0
5	sed_temp_mean	8.0	20.0	15.0

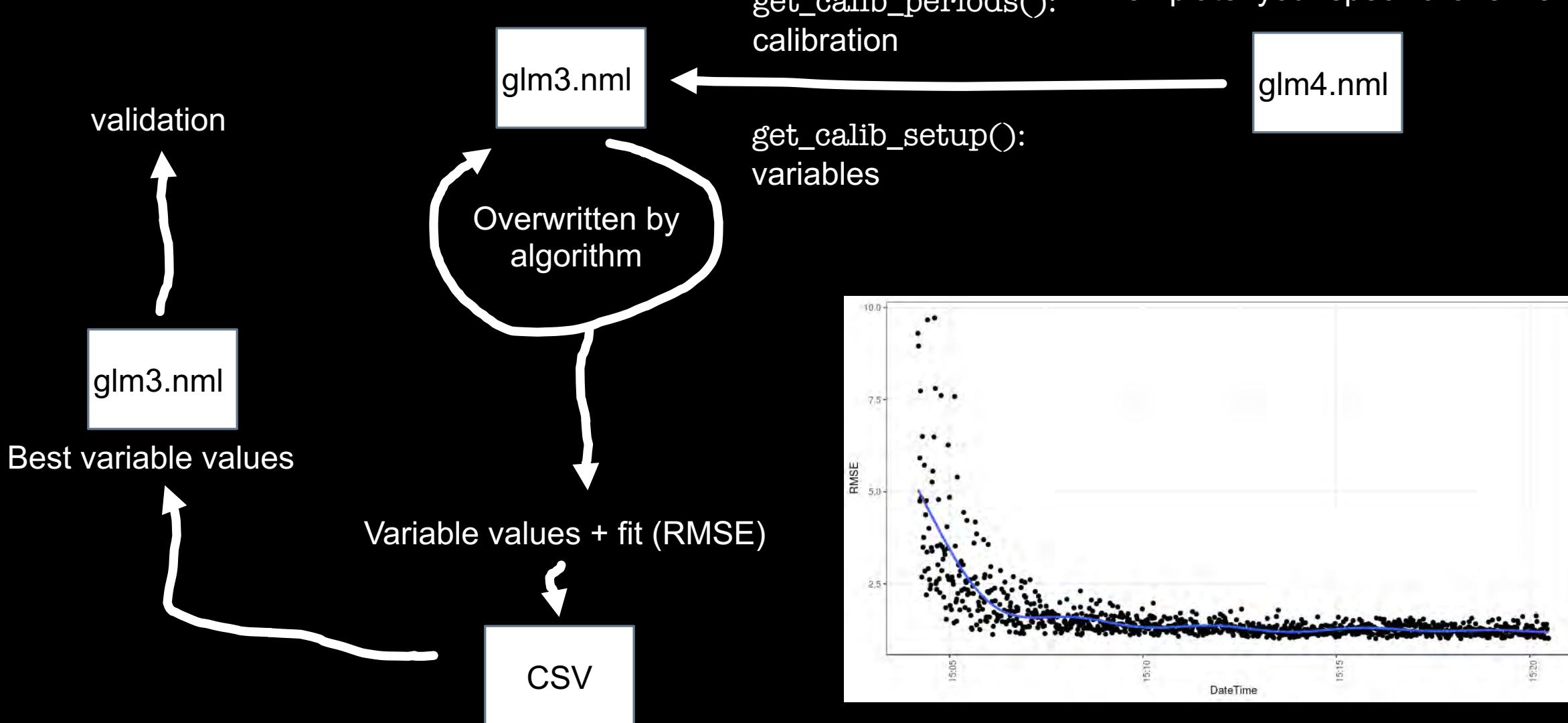
Sediment heat mean
temperatures to improve
vertical water temperature fit



Identified as sensitive by
global lake modeling
project ISIMIP

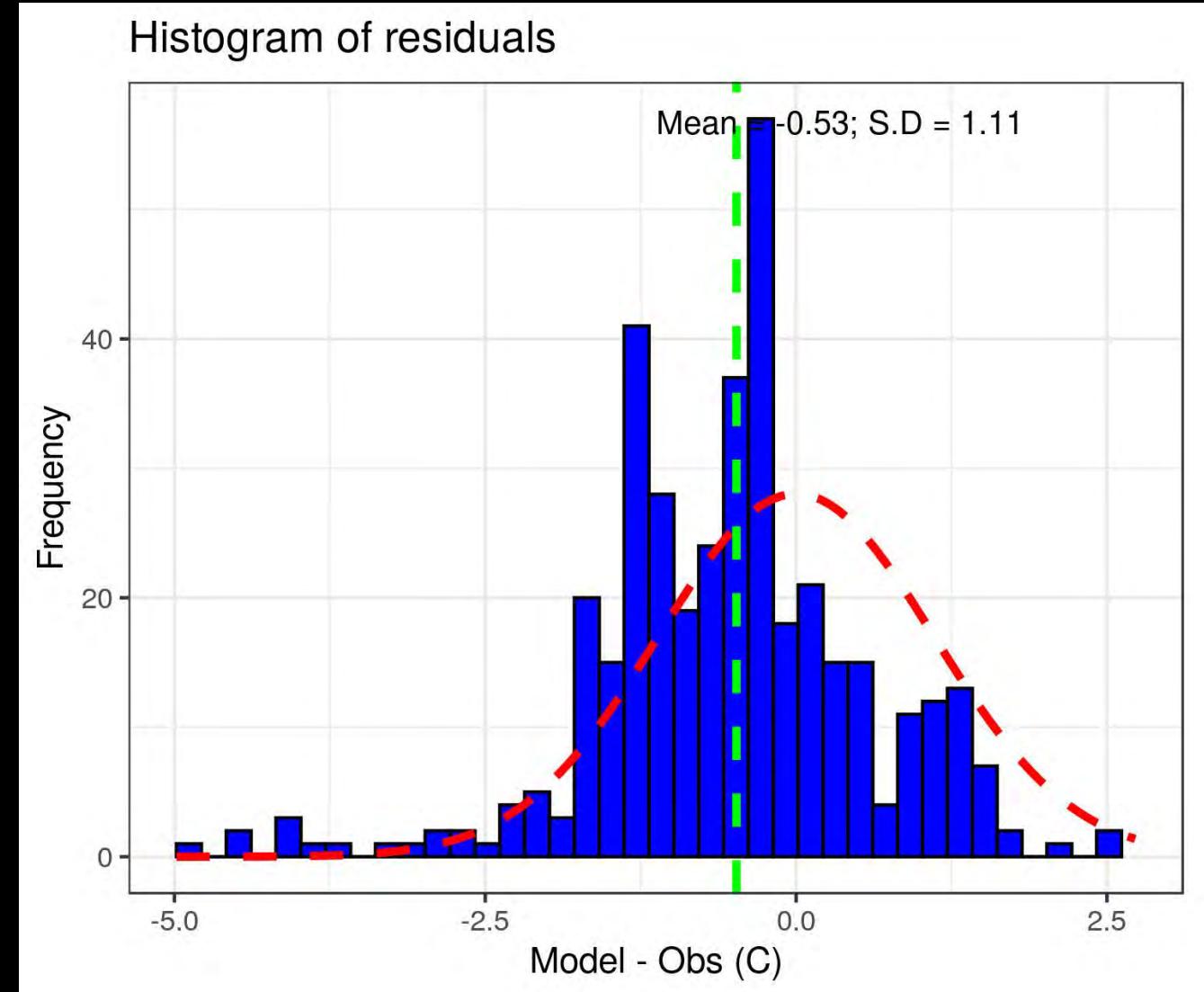


glmtools: calibration



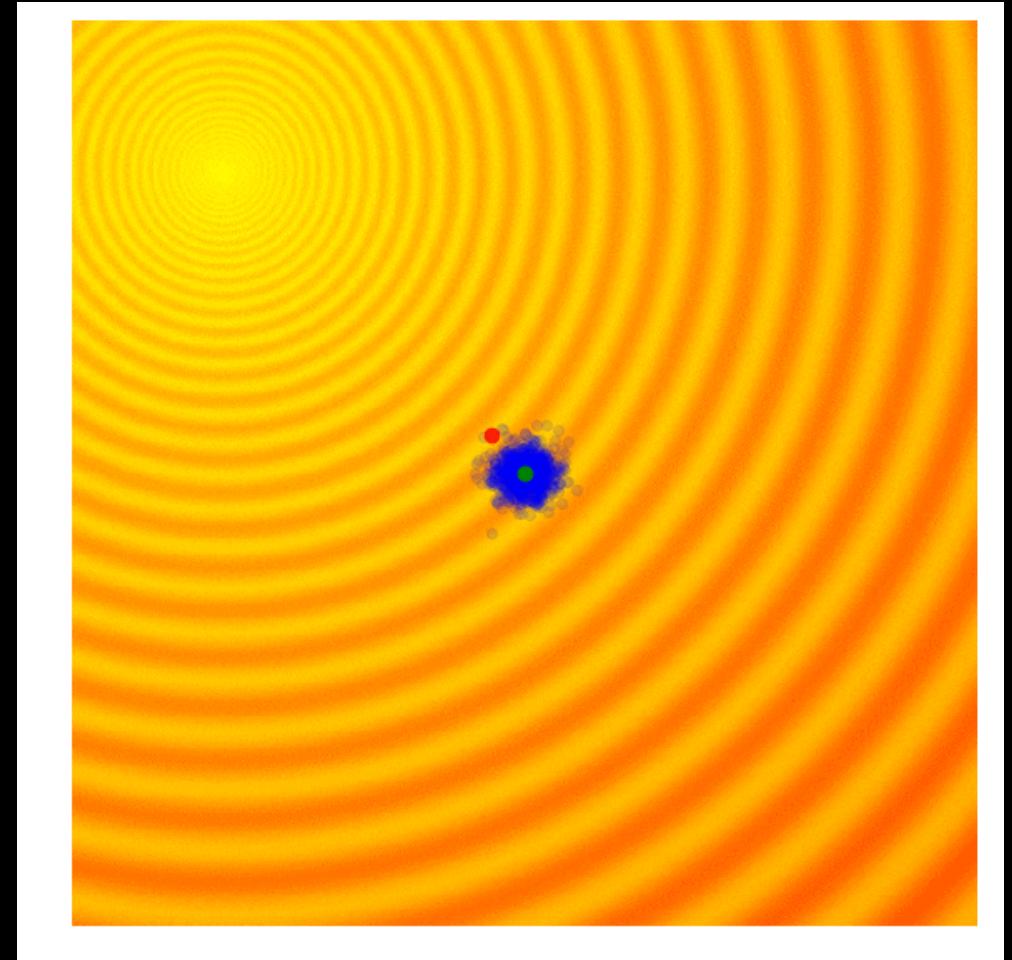
glmtools: calibration

- Calibration and validation as best practice
- Easy automatic calibration instead of manual tinkering
- Stored values in CSV give conclusions about parameter space
- Easier documentation

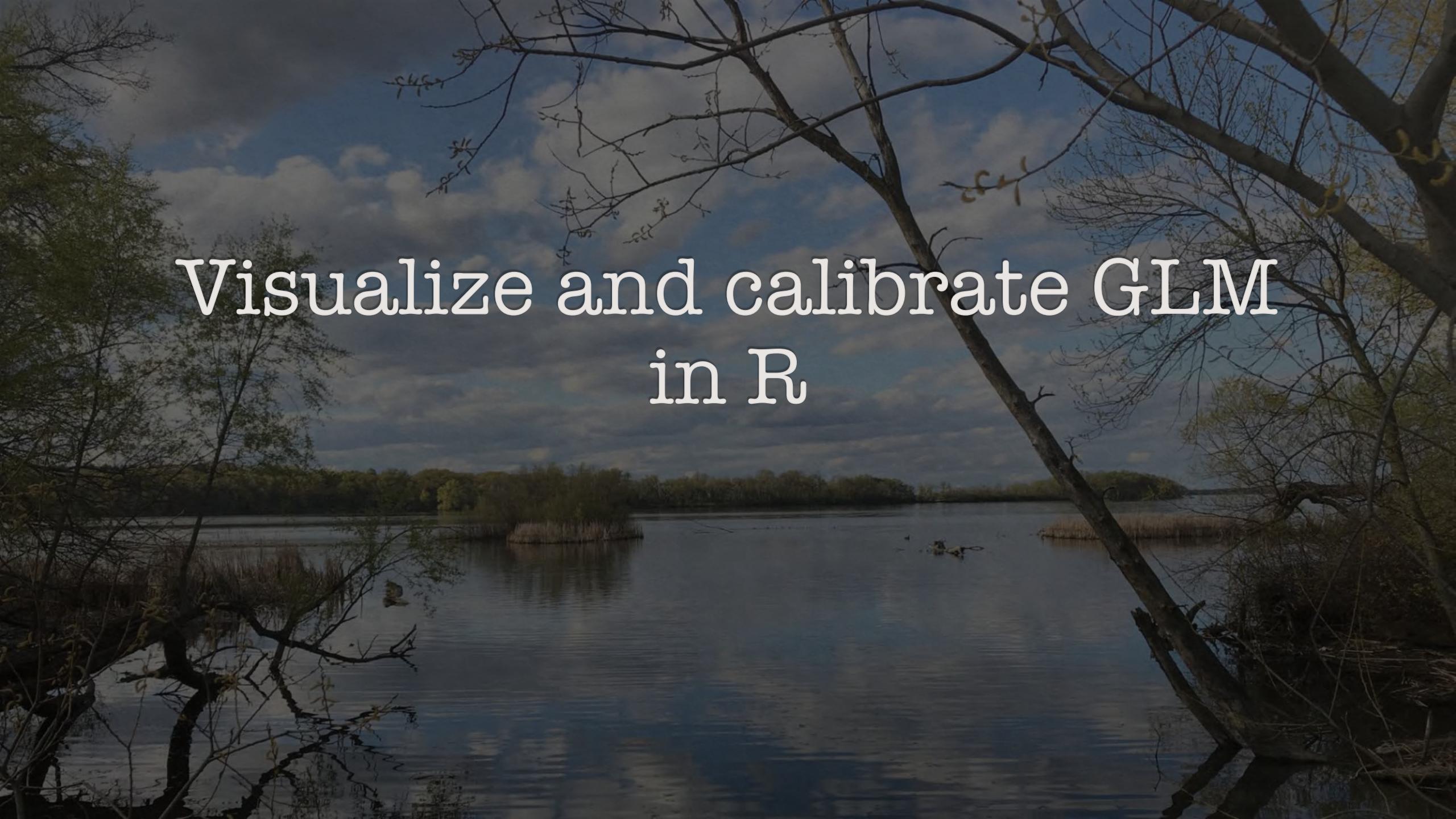


Evolutionary optimization (default)

- Optimization criteria: minimize RMSE between observed and modeled water temperatures
- CMA-ES (Hansen 2006)
 - Covariance Matrix Adaption - Evolution Strategy
 - Derivative-free optimization
 - 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 ($O(N^2)$)
- Stops after reaching certain RMSE (default 1.5 °C) or doing a finite amount of iterations (default is 150)

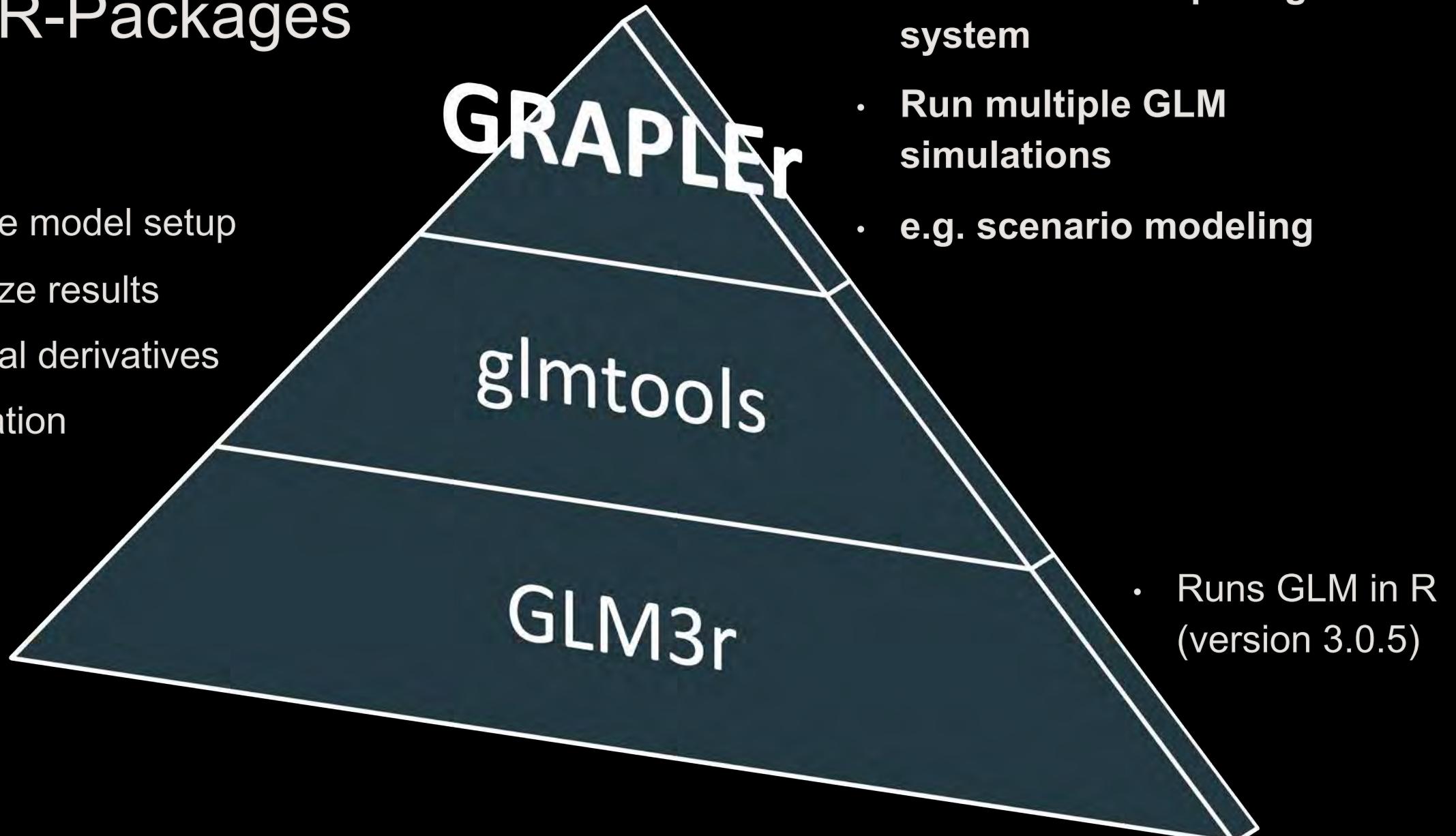


[Visual example \(link\)](#)



Visualize and calibrate GLM in R

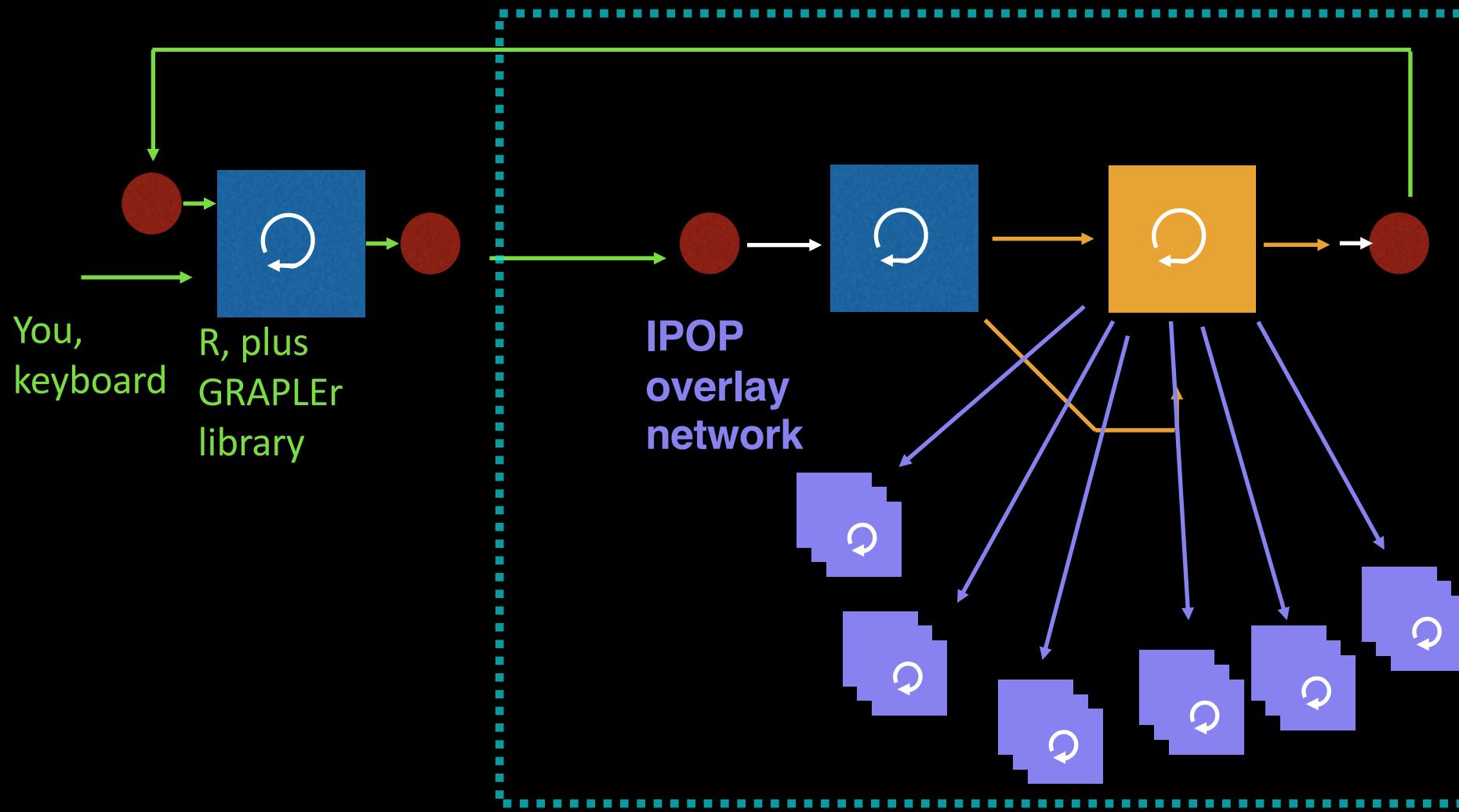
GLM R-Packages



GRAPLEr

- PRAGMA+GLEON inter-disciplinary expedition
 - <http://graple.org>
- Objective: allows you to run 1000s of GLM jobs
 - Dispatch to different computers across the Internet
 - Shorten execution times for large numbers of runs
- Distributed computing is not easy
 - GRAPLEr aims to facilitate access and use
 - Can submit jobs directly from R user interface

GRAPLER under the hood



GRAPLER Workflows

- Prepare GLM inputs to create an experiment
 - .nml, .csv driver files
- Create your own inputs on your computer, or have GRAPLER generate your inputs
 - E.g. add a random number between 0, 2 degrees Celsius to AirTemp, from a uniform distribution; add a constant, linear offset
- Optionally, add a post-processing filter (to reduce size of output)
- Submit experiment
 - From R, R-Studio
- Wait for completion, and download outputs

GLM R-Packages and where to find them



github

Development version
from `hdugan/glmtools`
will soon be merged
into official repository



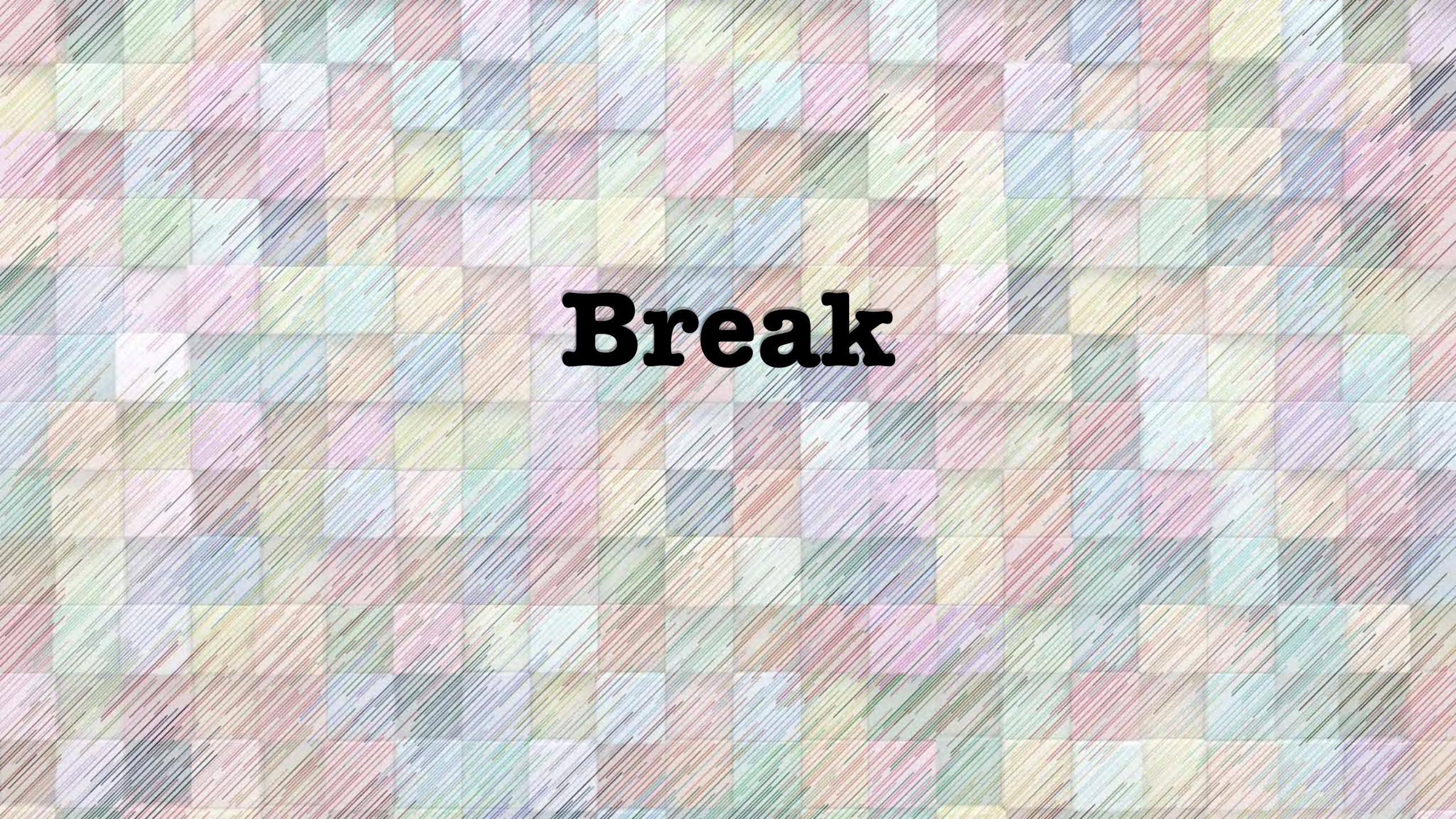
GRAPLE/GRAPLER

USGS-R/glmtools

GLEON/GLM3r

`library(devtools)`

`devtools::install_github()`



Break

Future development

- “**Containerized**” GLM:
 - Containers are standardized units of software (include code and dependencies)
 - standalone executable package
 - not depending on operating system
 - GLM-AED2 is available at dockerhub (hydrobert/glm-aed2)
 - Can be used in R:
https://github.com/robertladwig/GLM_docker
- Online-GLM: **columbus4limnology.io**
 - Share data and run GLM in the cloud!



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Demonstration



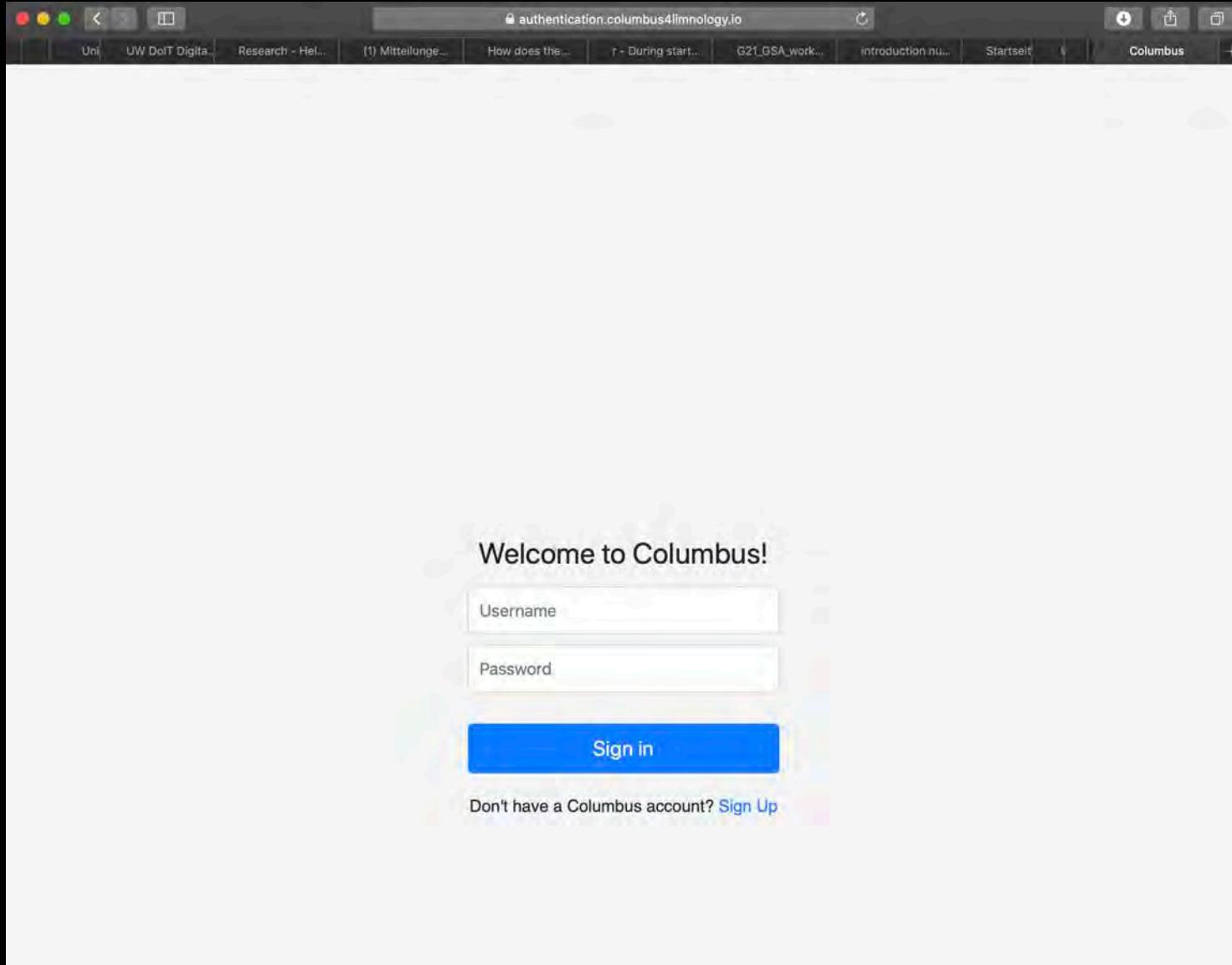


AnHai Doan
Prof. @ CS
UW-Madison

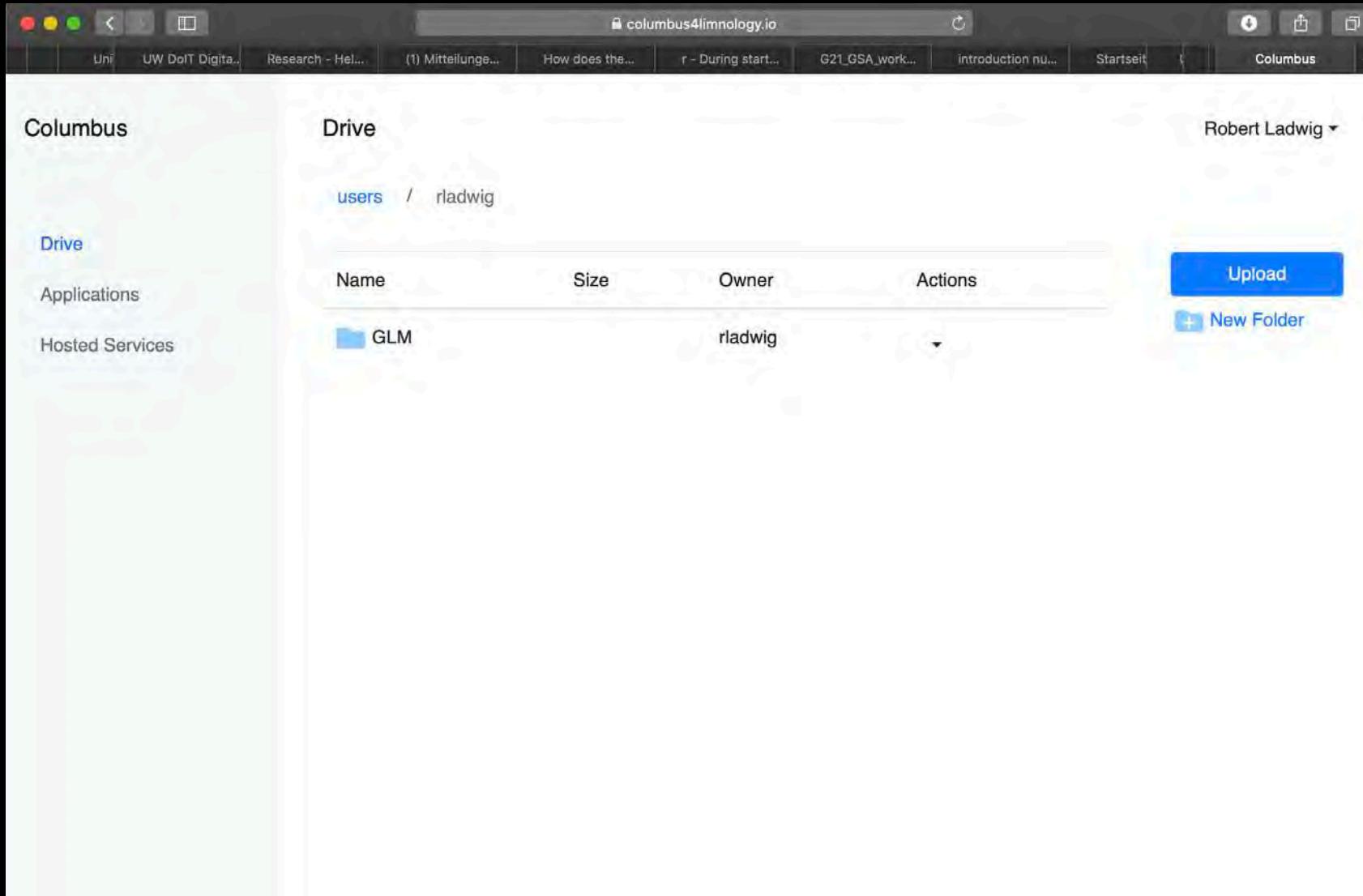
columbus4limnology.io

And his team, Amanpreet Singh Saini and Kaushik Chandrasekhar.
Funding in part through UW Data Science Initiative

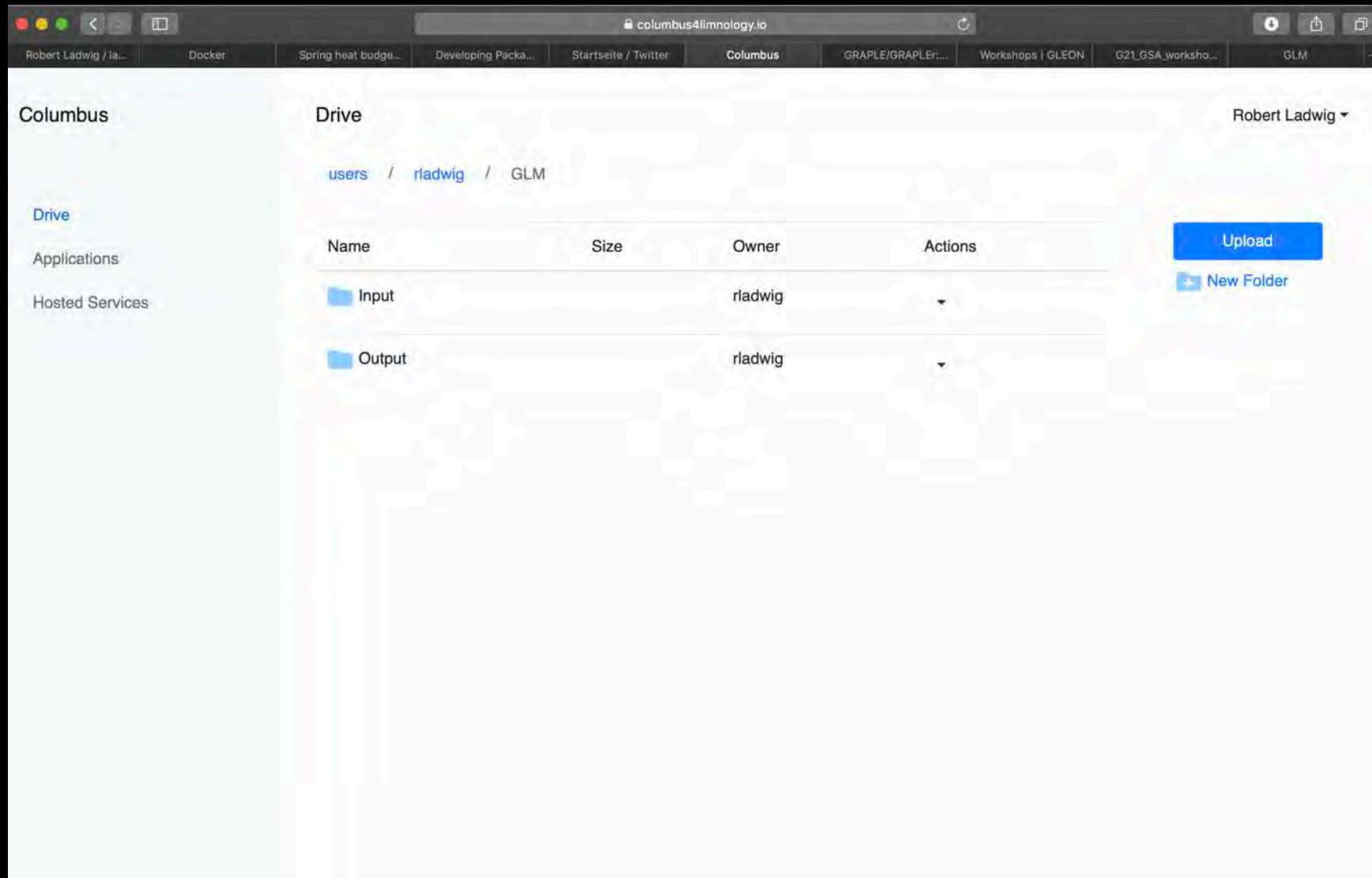
Create an account



Upload your model setup



Have two folders

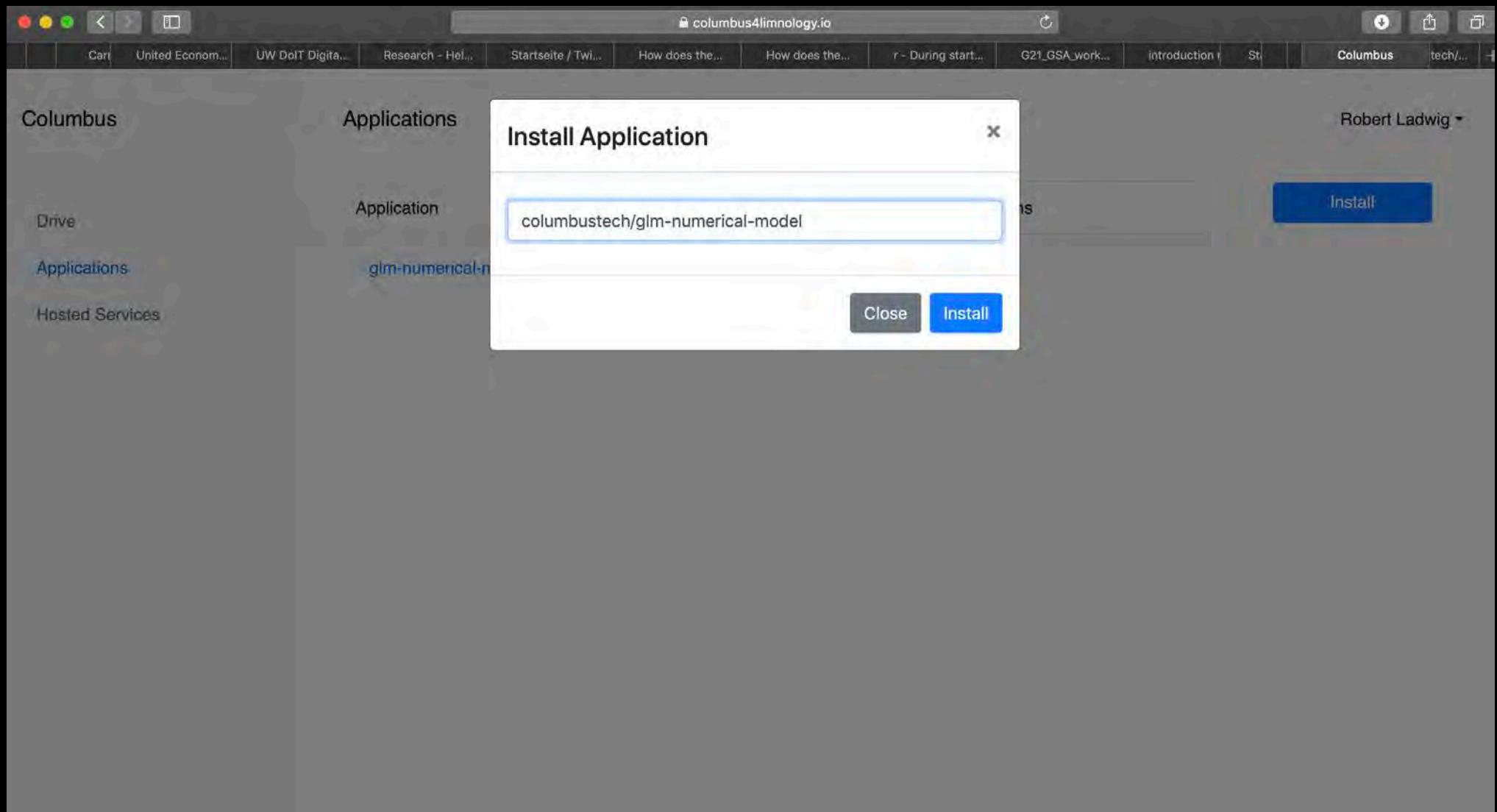


You'll need a glm3.nml file and driver data

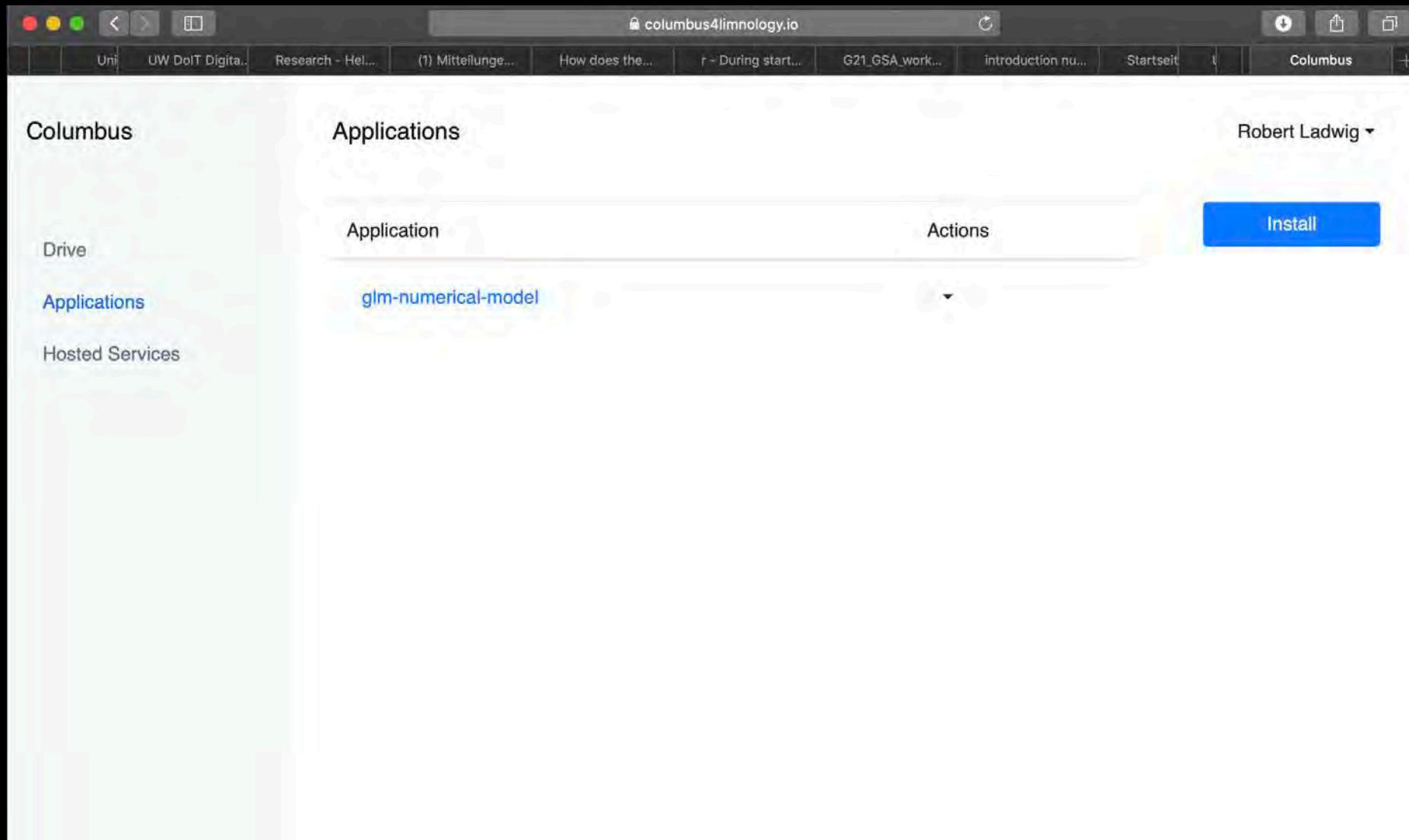
The screenshot shows a web-based file management interface titled "Columbus Drive". The URL in the address bar is "columbus4limnology.io". The navigation path is "users / rladwig / GLM / Input". On the left, there's a sidebar with "Drive", "Applications", and "Hosted Services" sections. The main area displays a table of files:

Name	Size	Owner	Actions
glm3.nml	3603	rladwig	Upload New Folder
met_driver.csv	1332425	rladwig	
aed2.nml	15208	rladwig	

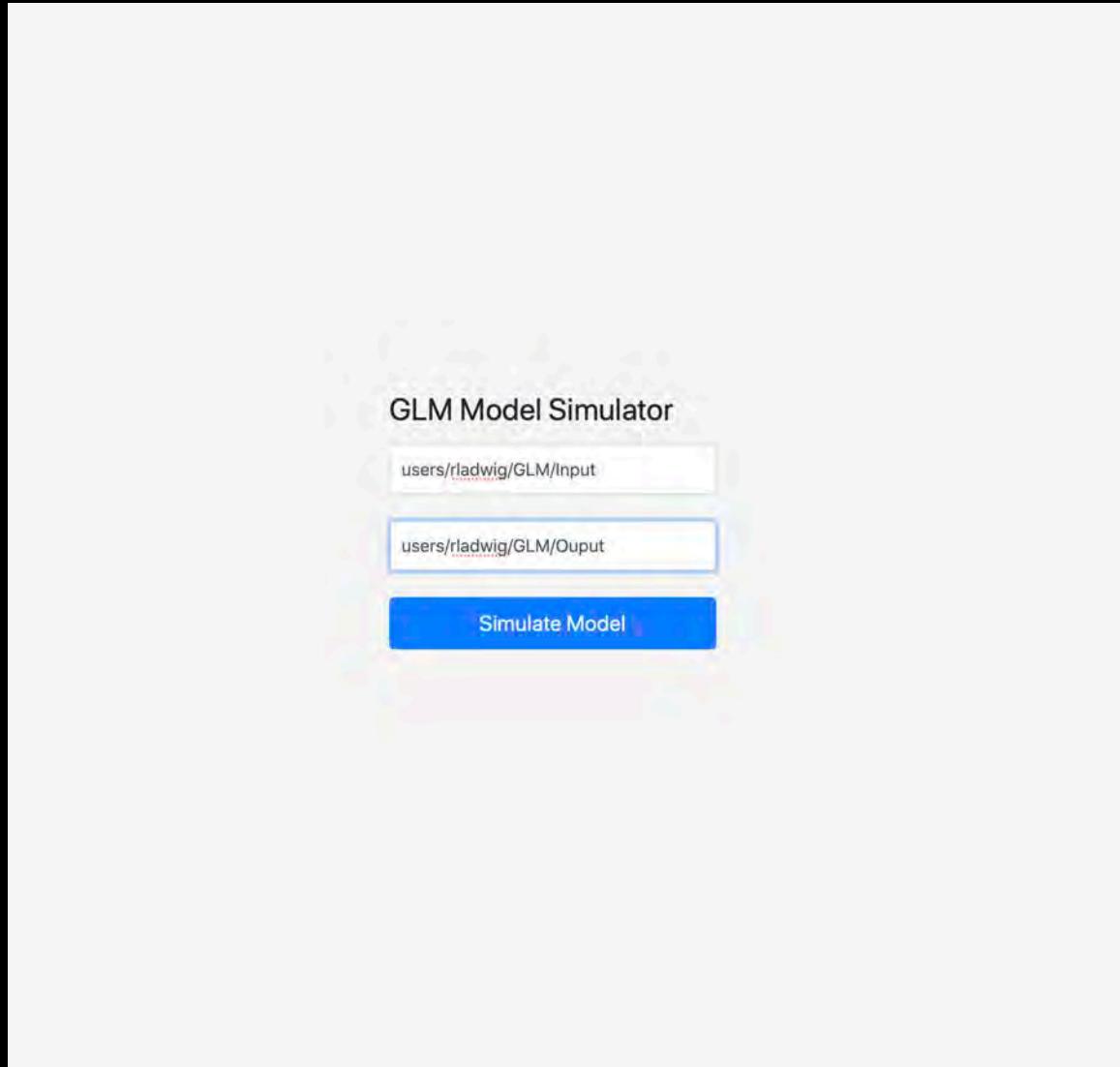
Install the docker container



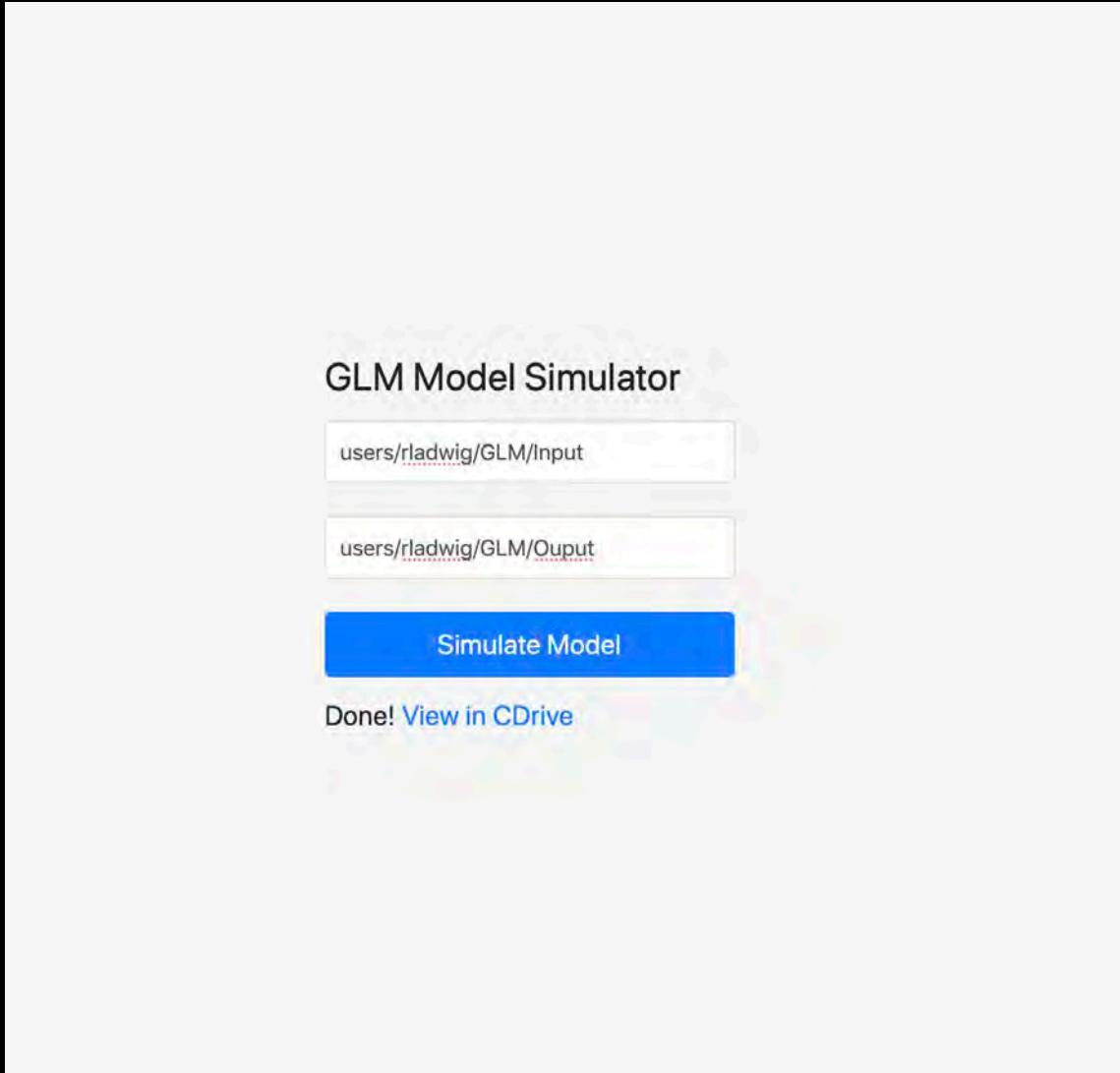
Click on the application



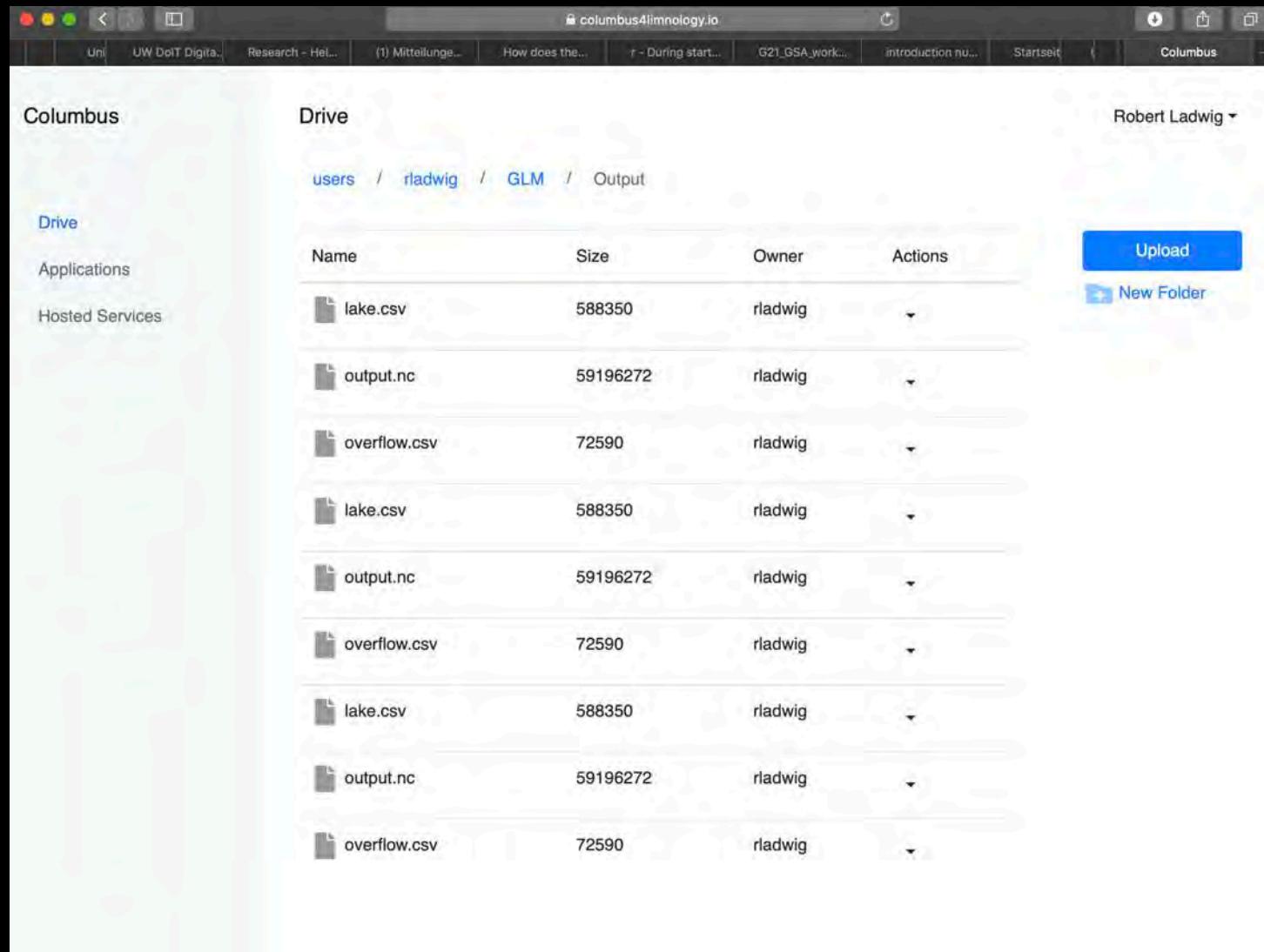
Type in the input and output paths



Simulate model



Download the output



columbus4limnology.io

- Feel free to create an account and to run GLM simulations in the cloud!
- You can share your model data with other users
- Hopefully this will enhance collaborations, and will help in finding mistakes in the model setup
- Containerized GLM could be a very flexible tool



Join the GLM community

- Find latest source code at
<https://github.com/AquaticEcoDynamics/GLM>
- Here, you can raise issues (errors, compilation problems, suggestions, improvements, bugs)

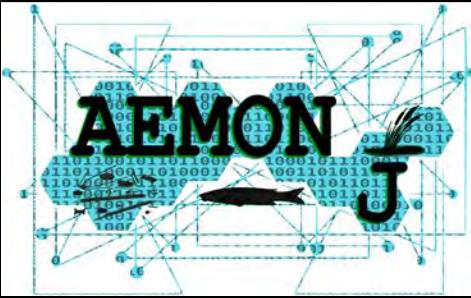
A screenshot of the GitHub repository page for AquaticEcoDynamics / GLM. The 'Issues' tab is circled in red. The page displays 9 open issues, 3 pull requests, 1 project, 1 wiki page, 1 security issue, and 13 forks. It also shows 74 commits, 1 branch, 2 releases, 4 contributors, and the GPL-3.0 license. A list of recent commits is listed below:

Commit	Description	Date
casper-boon bug fixes - (#18) and bad index in mobility	build improvements for win and os-x	2 years ago
.travis	bug fixes - (#18) and bad index in mobility	16 days ago
debian	version 3 release candidate 1	11 months ago
include	minor time fix, some tidying	2 months ago
macos	fixed minor issue with inflow	2 months ago
patches	bug fixes - (#18) and bad index in mobility	16 days ago
src	bug fixes - (#18) and bad index in mobility	16 days ago
win	bug fixes - (#18) and bad index in mobility	16 days ago
versionnumber_update	version number update	2 months ago

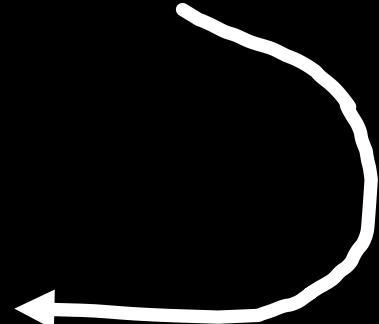
- Old: google group (forum)
<https://groups.google.com/forum/#!categories/aquaticmodelling/glm>
- New: **slack**



Join



- **Network for early career scientists**
- Focus on modeling of aquatic ecosystems
- Annual workshops (Australia, Ireland)
- Meeting during GLEON
- Join our **slack** to find collaborations, ask questions and complain about research



[aemon-j / aquatic-ecosystem-model-library](#)

Code Issues Pull requests Projects Wiki Security Insights

Home
Robert Ladwig edited this page on Sep 25, 2018 · 8 revisions

Welcome to the Aquatic Ecosystem Model Library!

This is a wiki created by the AEMON-J network for developing/documenting the existing aquatic ecosystem models. Our intention is to create an interactive platform to help new modellers to choose the models that suit their needs, and to attract more advanced modeller to input their modelling knowledge.

For navigation, take a look at the side bar on the right margin of this page.

For more information about AEMON-J please visit the [google forum](#) and get involved, or the [AEMON website](#) for news and resources.

If you have questions, suggestions, criticism or want to know even more, don't hesitate and contact us via aemonj.models@gmail.com.

+ Add a custom footer

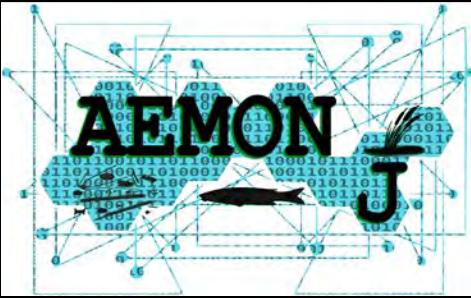
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- AED2
- al2water
- CAEDYM
- DYRESM
- FABM-PCLake
- FLake
- GOTM
- GLM
- MyLake
- MGNERIS
- PCLake/PCLake+
- SALMO
- Simstrat



Next AEMON workshop



- ASLO 2020 in Madison, WI (USA)
- June 7 – 12, 2020
- Probably the weekend before
- Travel support is possible (lodging and meals)
- More information as soon as possible



Thank you

- Find latest source code at
[https://github.com/AquaticEcoDynamic
s/GLM](https://github.com/AquaticEcoDynamic/s/GLM)
- Here, you can raise issues (errors,
compilation problems, suggestions,
improvements, bugs)
- Join GLM slack to ask questions and
get

