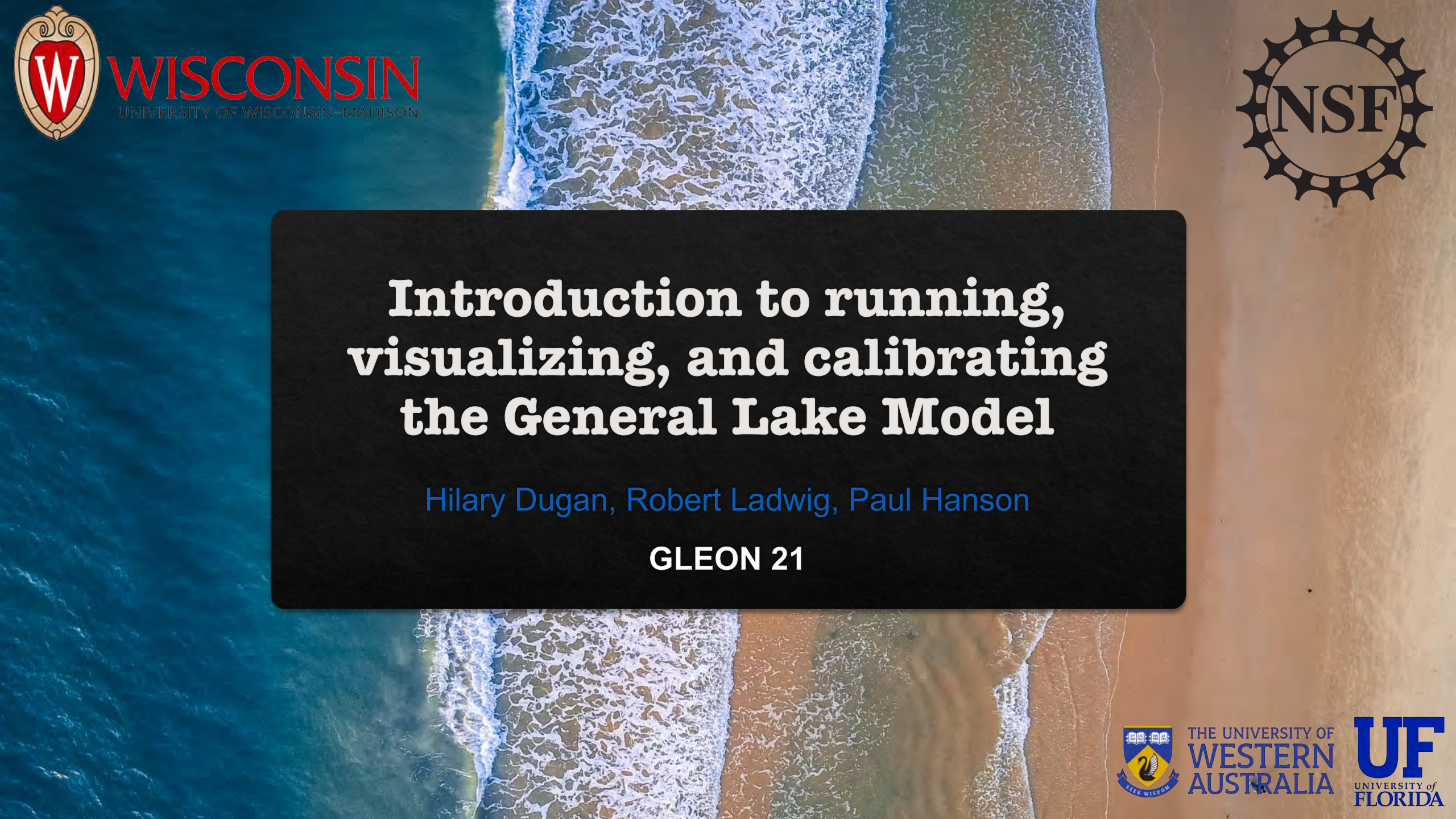


Introduction to running, visualizing, and calibrating the General Lake Model

Hilary Dugan, Robert Ladwig, Paul Hanson

GLEON 21

Find all material and data here

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

Who some of us are

Hilary Dugan
Assist. Prof. @ CFL
UW-Madison

Paul C. Hanson
Research Prof. @ CFL
UW-Madison

Matt Hipsey
Assoc. Prof. @ AED
UWA Perth

Renato Figueiredo
Prof. @ ESE
Univ. of Florida

Robert Ladwig
Postdoc @ CFL
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?

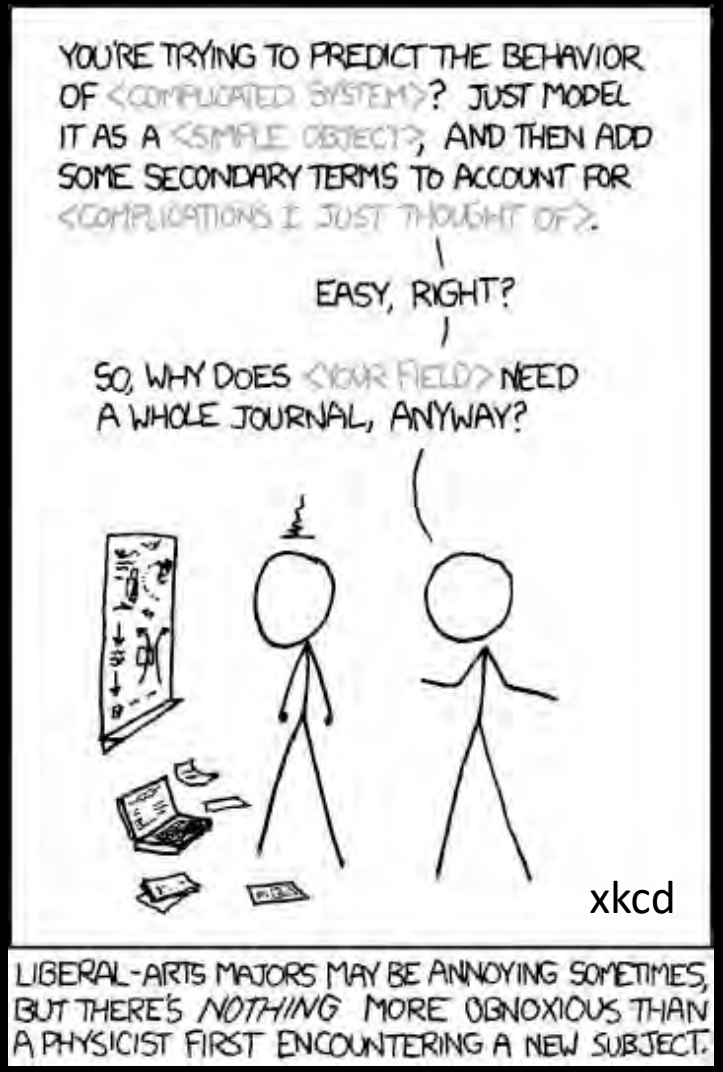
Scope of this workshop

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

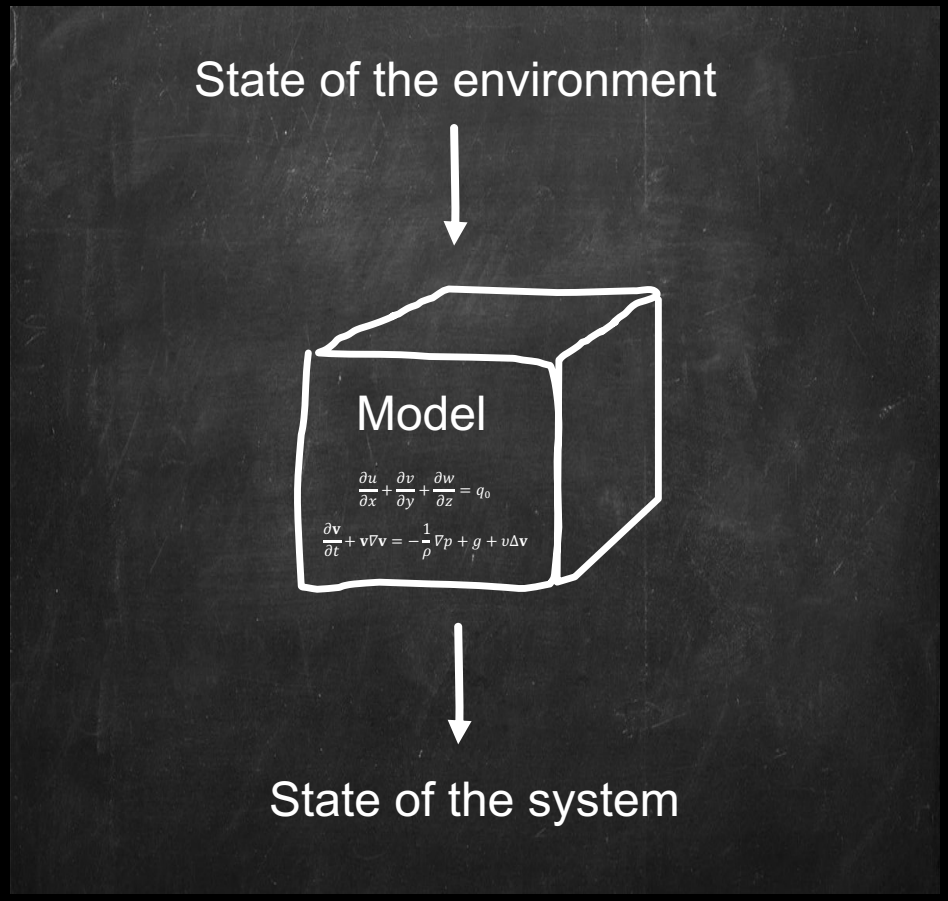
- Models are simplified reflections of reality
- Deterministic (events at next time step depend on events from previous time step)
  - and describe processes with mathematical equations
  - that are either based on empirical knowledge or physical principles

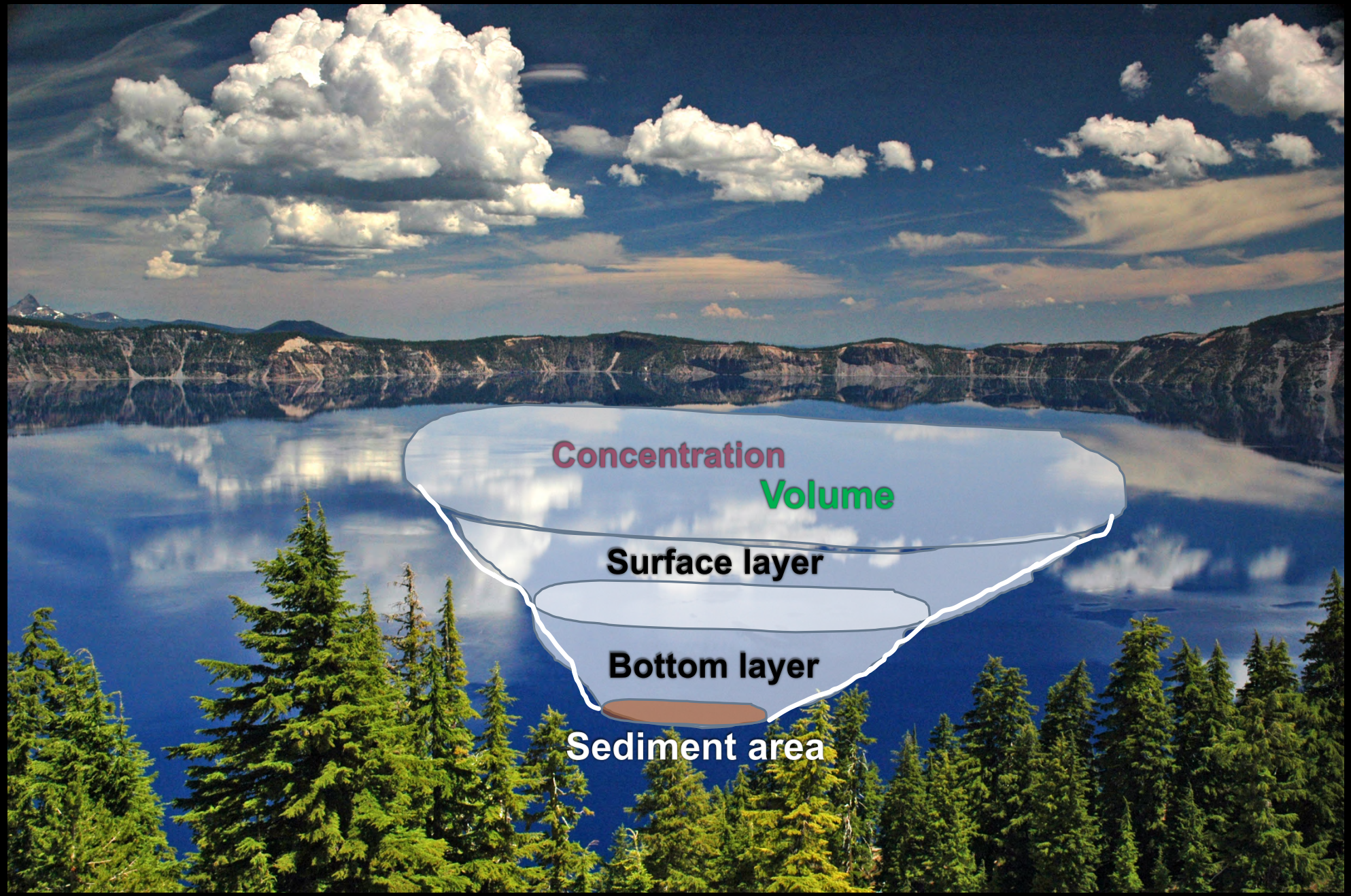
- Numerical models need time and space discretization
- As well as initial data (to start from) and boundary data (as driving data)



Crash course: Numerical Modeling

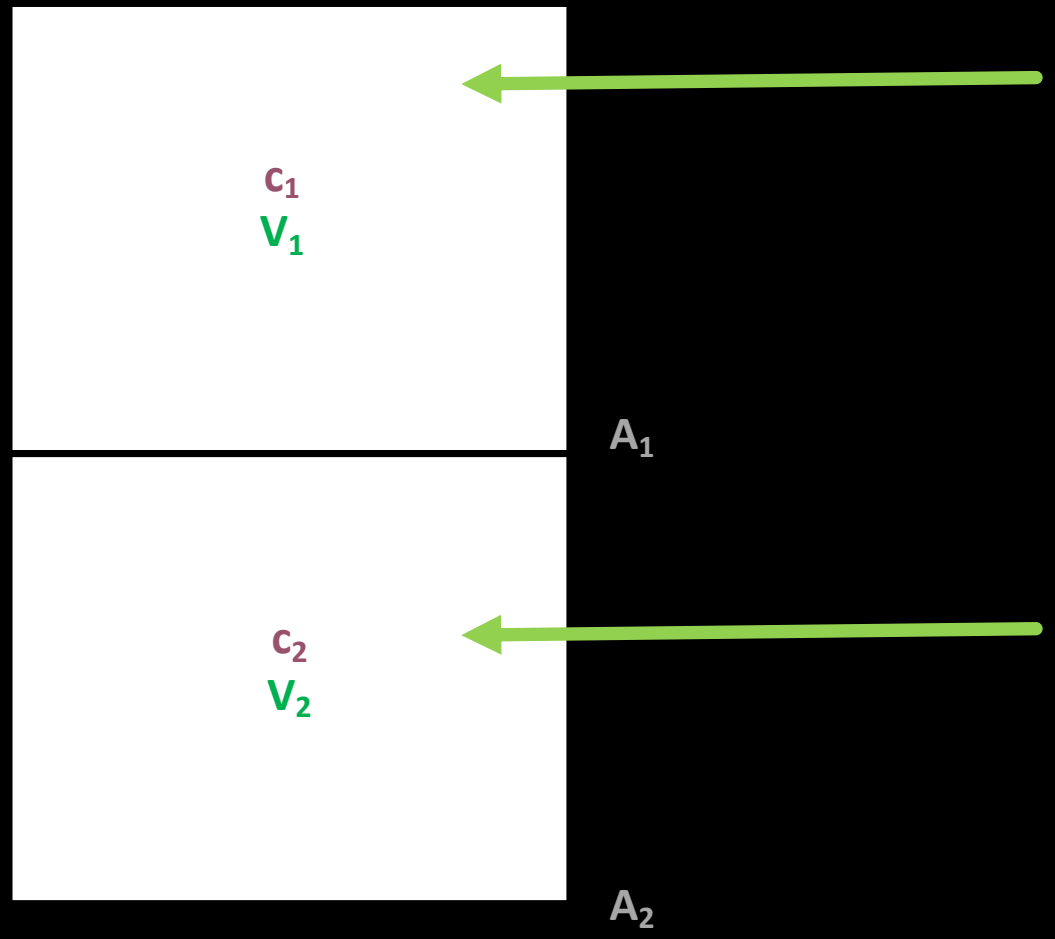
- **Conservation of mass (continuity)**
  - Inflow(s)= outflow(s)
  - Mass cannot be created or destroyed
- **Conservation of momentum**
  - Velocity based on balances of forces (gravity, pressure, friction, earth-rotation)





Crash course: Numerical Modeling

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



Surface layer

Concentration

Volume

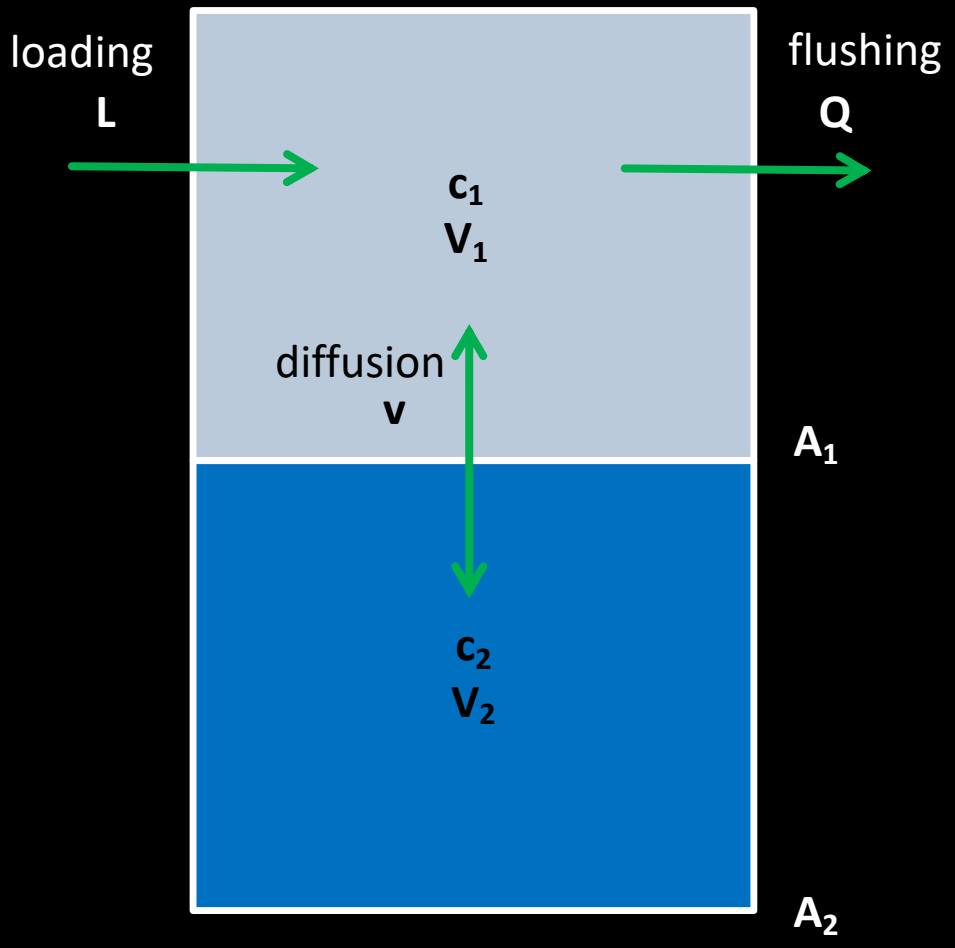
Area dividing the two zones

Bottom layer

Sediment area

Crash course: Numerical Modeling

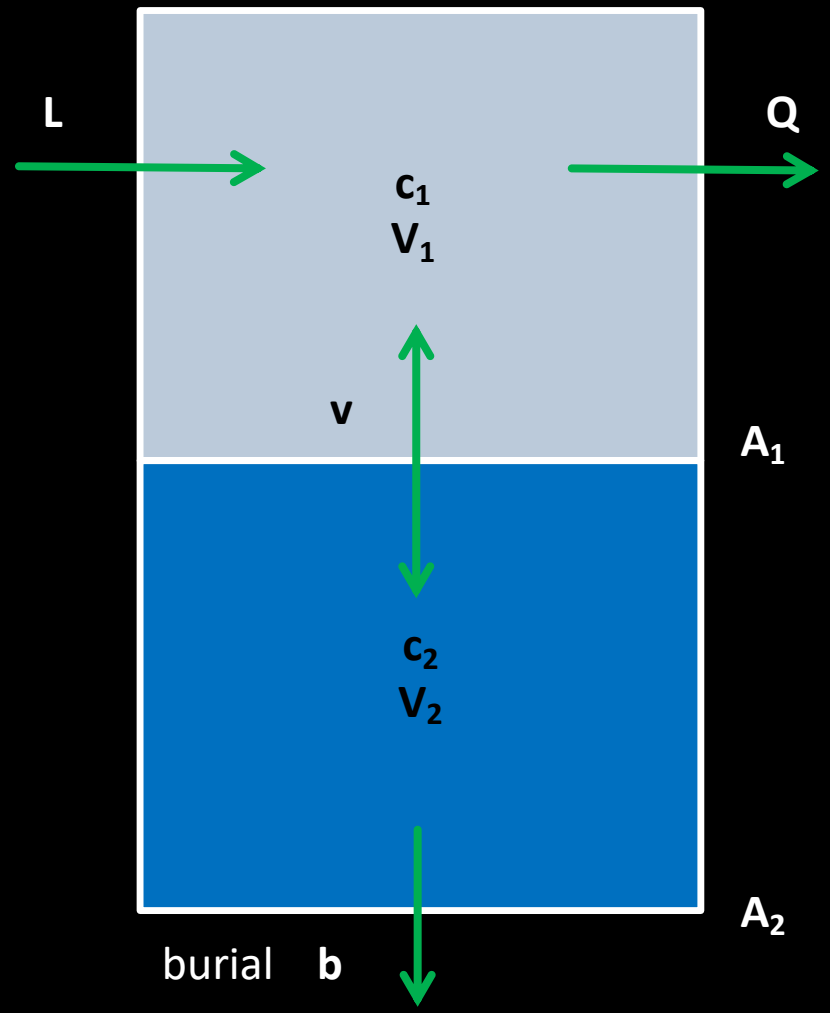
Most are bookkeeping exercises to keep inflow = outflow (mass-balance)



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

Crash course: Numerical Modeling

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

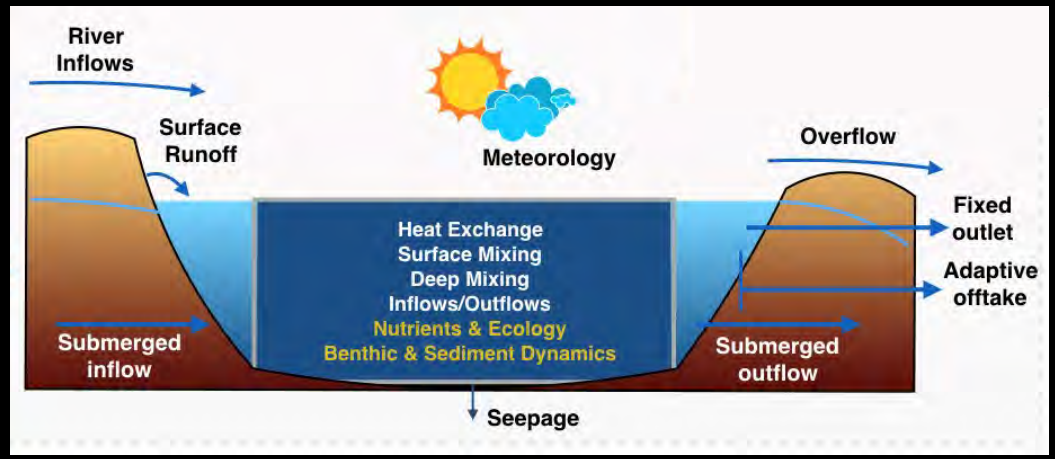


$$\frac{dc_1}{dt} = \frac{L - Qc_1 + vA_1(c_2 - c_1)}{V_1}$$

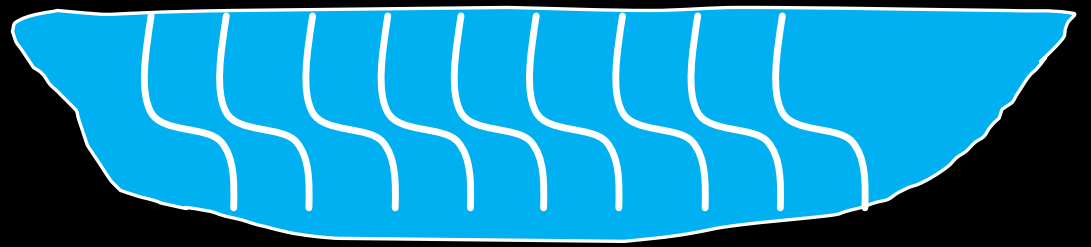
$$\frac{dc_2}{dt} = \frac{vA_1(c_1 - c_2) - bA_2c_2}{V_2}$$

Introduction to GLM

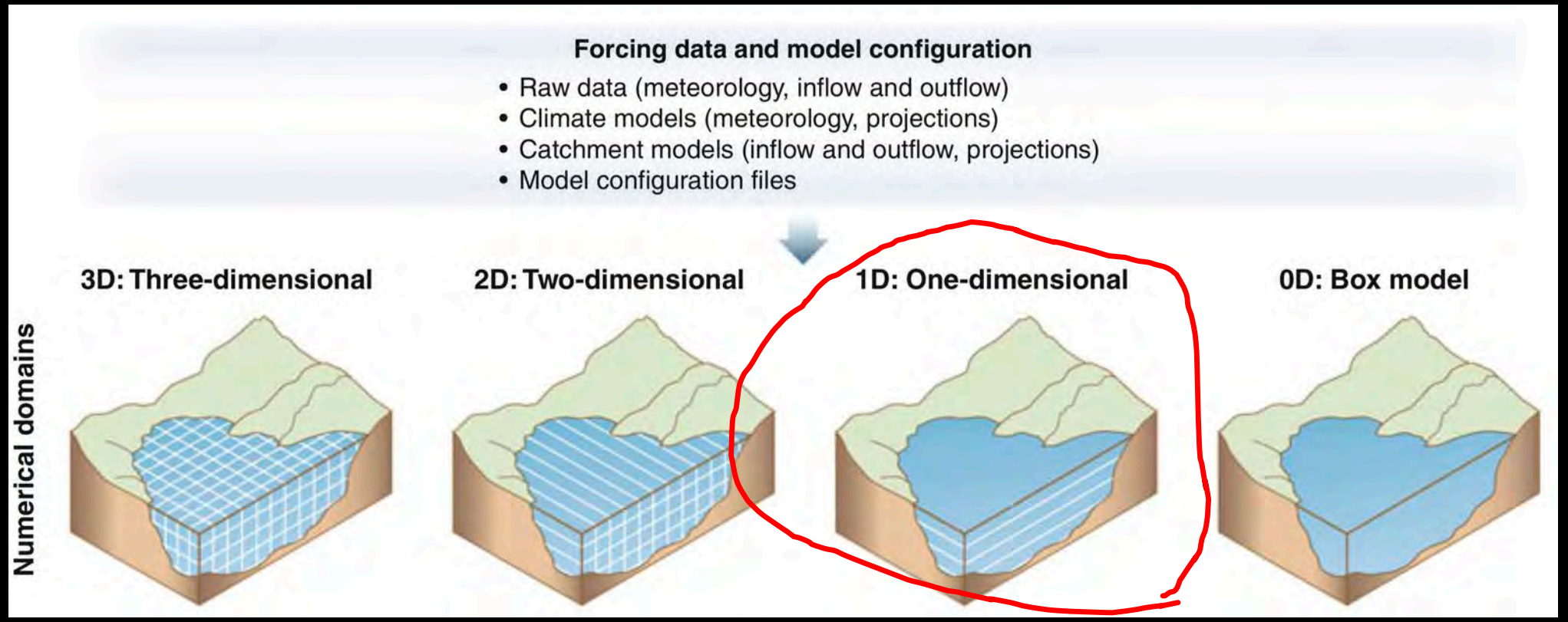
- Supported as a project within GLEON
- Developed by Matt Hipsey, Louise Bruce and Casper Boon at UWA
- Designed to operate with the Aquatic EcoDynamics Model Libraries (AED) → water quality model
- Languages: C (and Fortran for AED)
- Freely available as open-source program
- https://github.com/AquaticEcoDynamics/GLM



Introduction to GLM

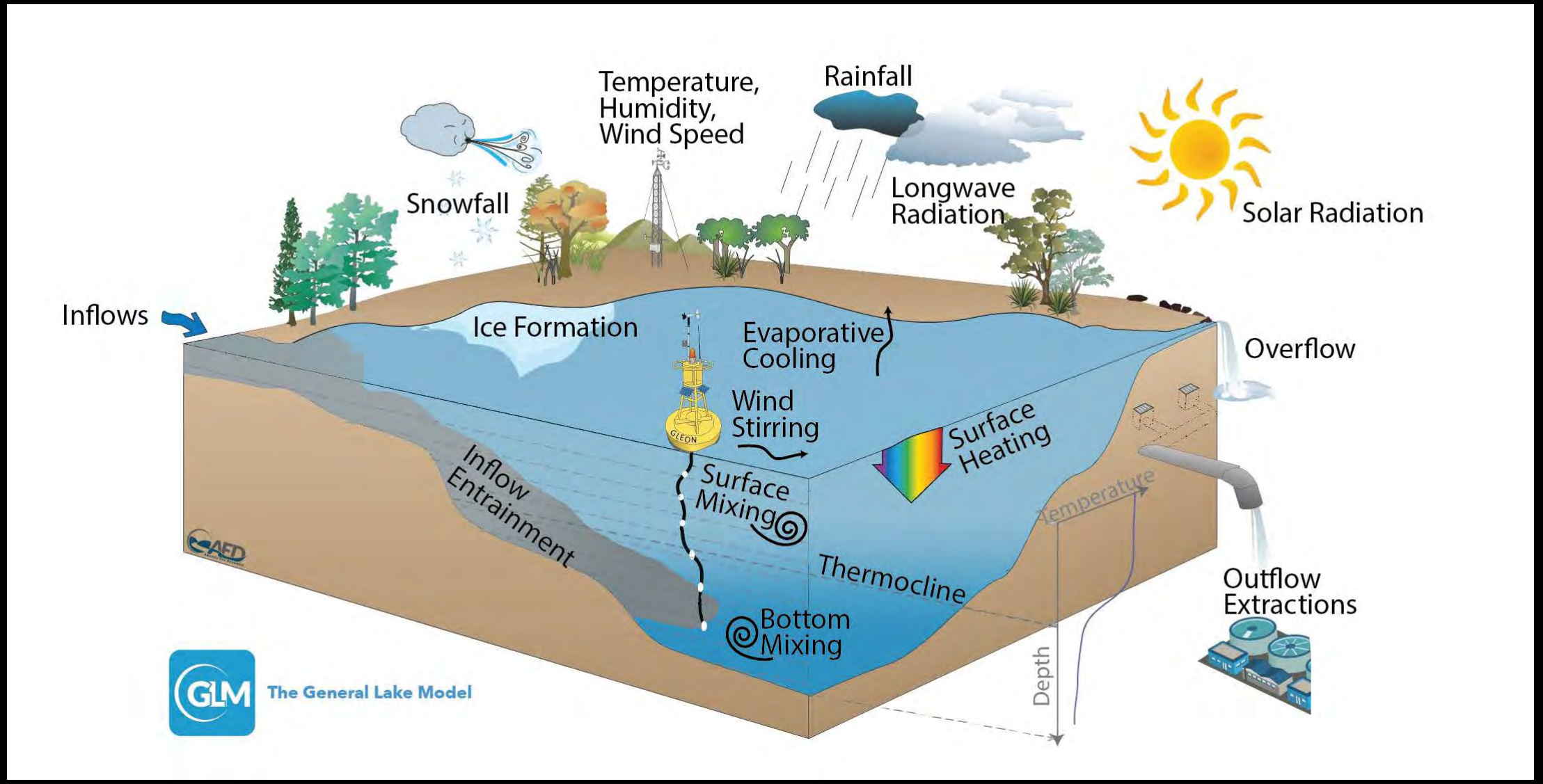


- Vertical one-dimensional model (spatially homogenous lake)



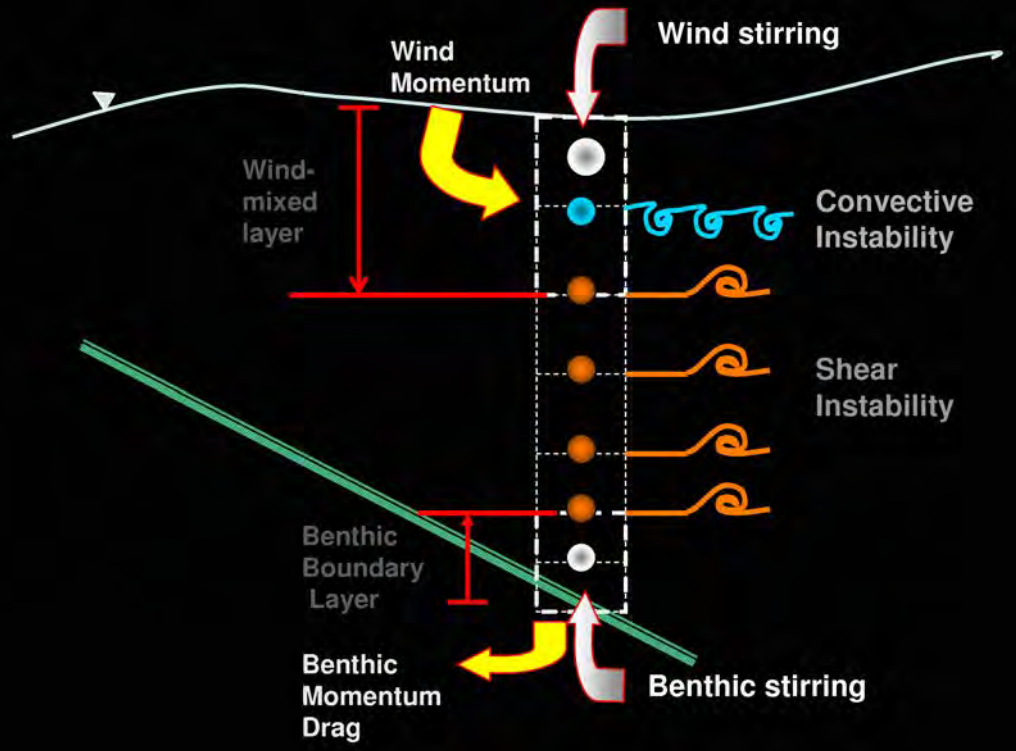
Trolle (2012)

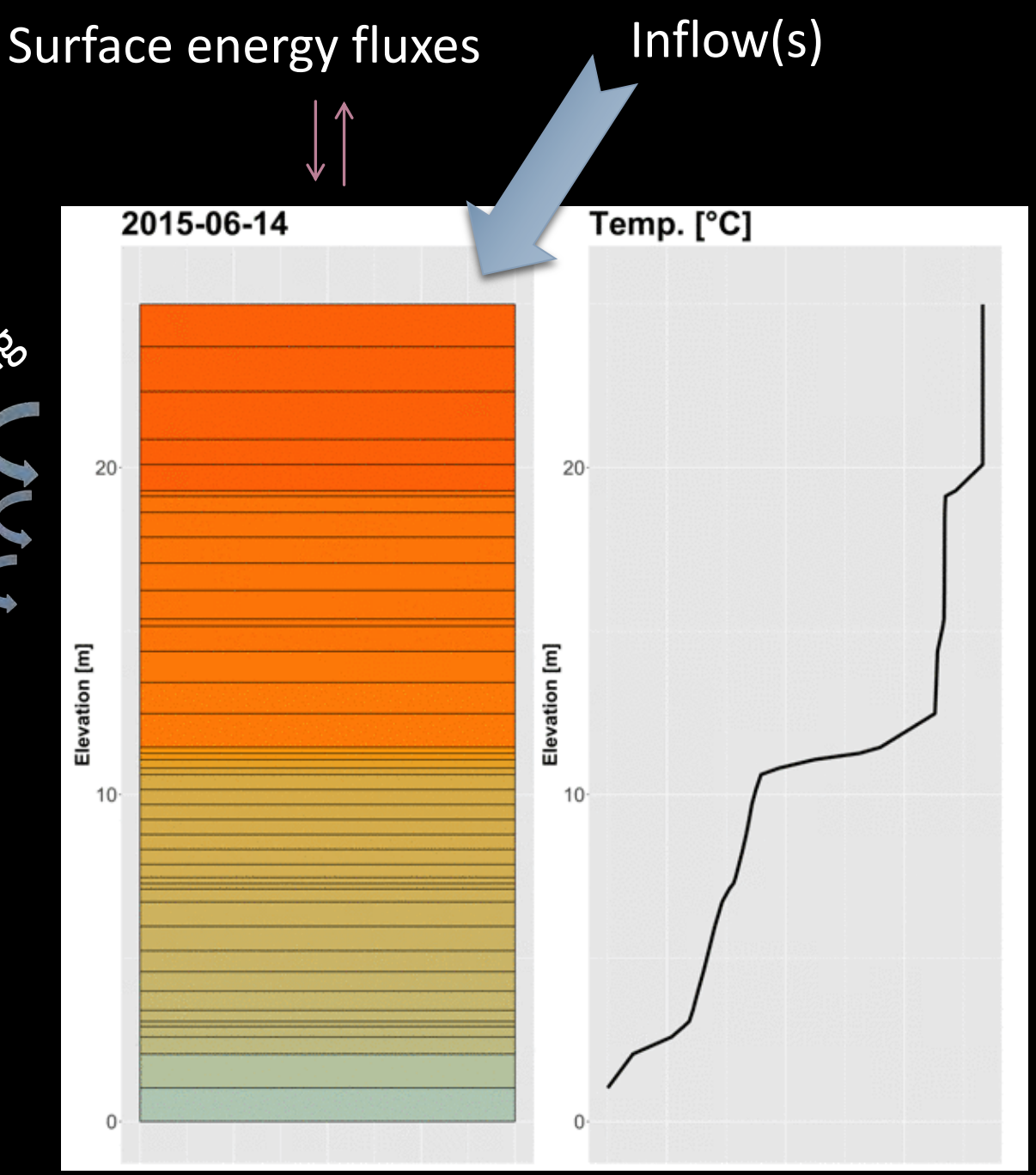
Introduction to GLM



Introduction to GLM

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





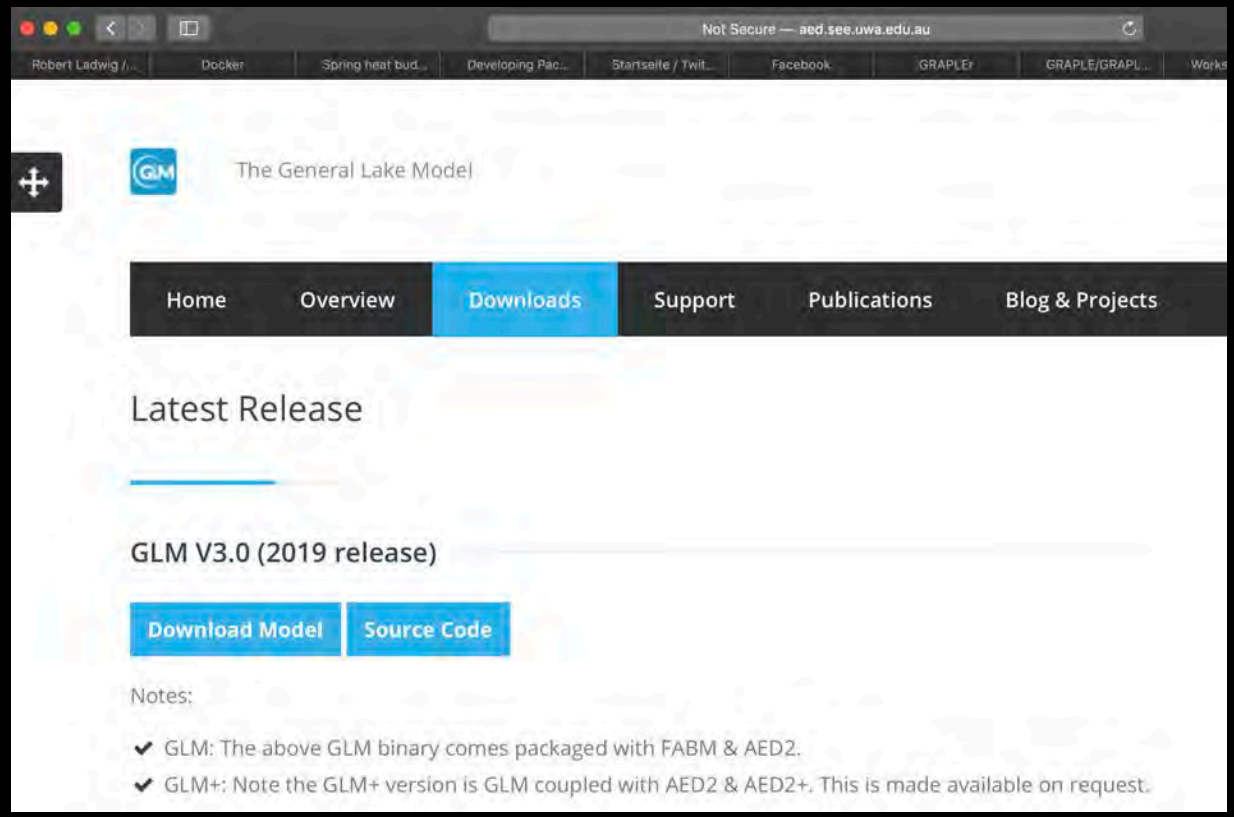
Introduction to GLM

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

```
!-----------------------------------------------------------------------------
! 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
!-----------------------------------------------------------------------------
```

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

```
!-----------------------------------------------------------------------------
! 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
!-----------------------------------------------------------------------------
```

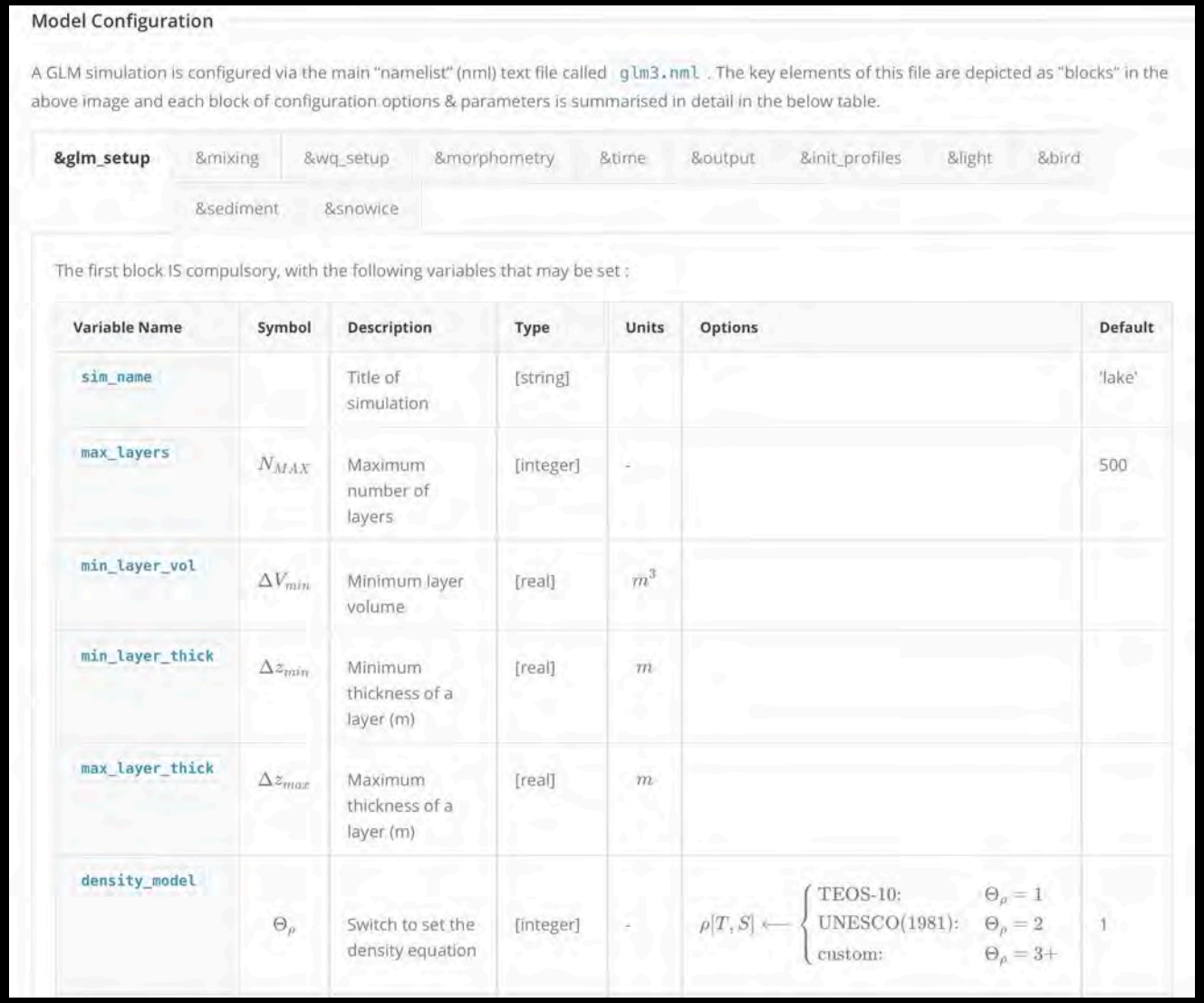
Introduction to GLM : setting up your model

1. Define the morphometry
    1. Area-depth relationship (hypsography)
2. Define what you want to simulate
    1. State variables (temperature, salinity, etc.)
    2. Grid resolution and time step
3. Define external environment
    1. Boundary conditions (inflows, meteorology, outflows)
4. Provide an initial condition
5. 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

Introduction to GLM : setting up your model



Model Configuration

A GLM simulation is configured via the main "namelist" (nml) text file called `glm3.nml` . 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 &light &bird &sediment &snowice

The first block IS compulsory, with the following variables that may be set :

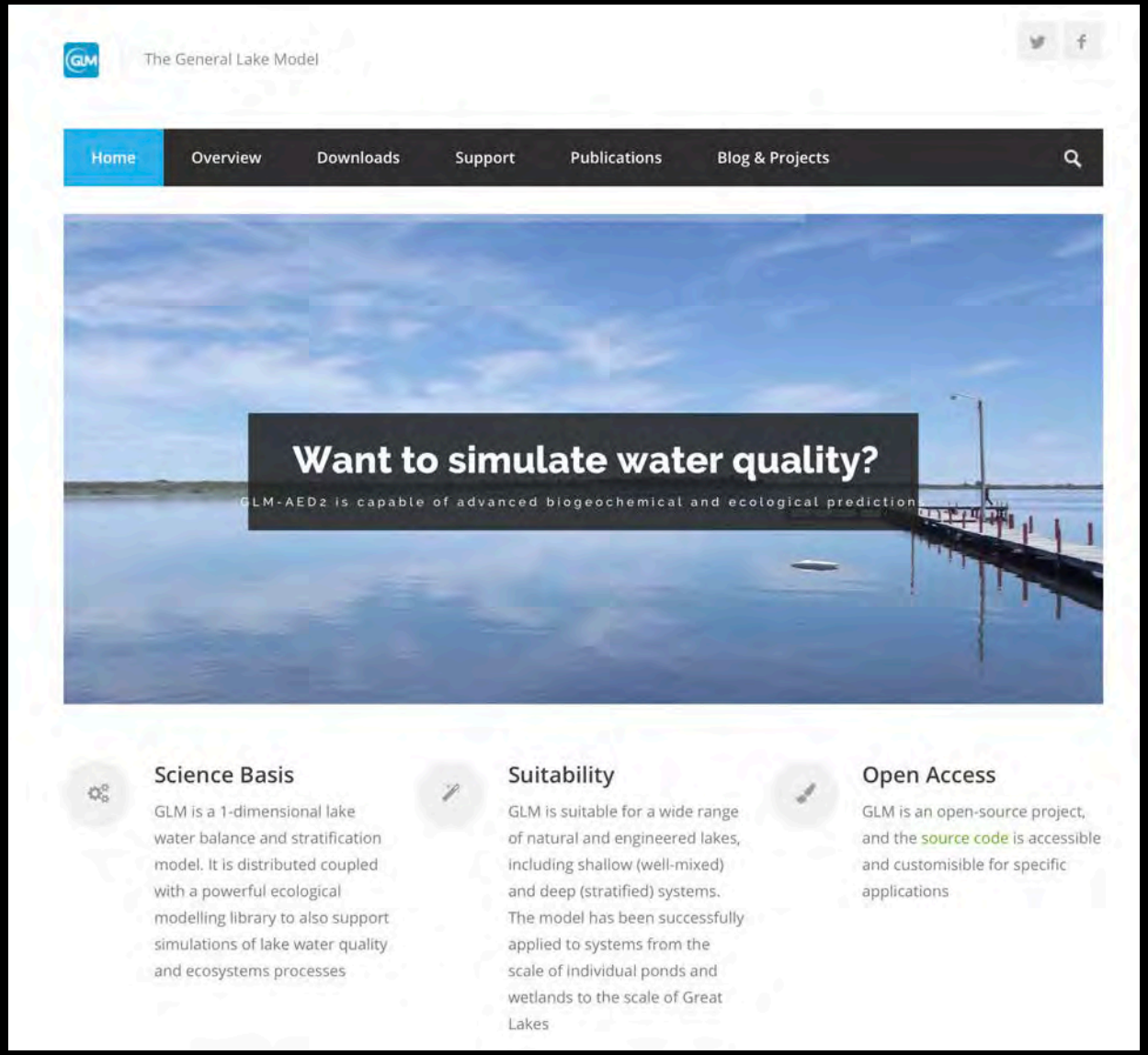
Variable Name	Symbol	Description	Type	Units	Options	Default
`sim_name`		Title of simulation	[string]			'lake'
`max_layers`	N_{MAX}	Maximum number of layers	[integer]	-		500
`min_layer_vol`	ΔV_{min}	Minimum layer volume	[real]	m^3		
`min_layer_thick`	Δz_{min}	Minimum thickness of a layer (m)	[real]	m		
`max_layer_thick`	Δz_{max}	Maximum thickness of a layer (m)	[real]	m		
`density_model`	Θ_ρ	Switch to set the density equation	[integer]	-	$\rho[T,S] \longleftarrow \begin{cases} \text{TEOS-10:} & \Theta_\rho = 1 \\ \text{UNESCO(1981):} & \Theta_\rho = 2 \\ \text{custom:} & \Theta_\rho = 3+ \end{cases}$	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

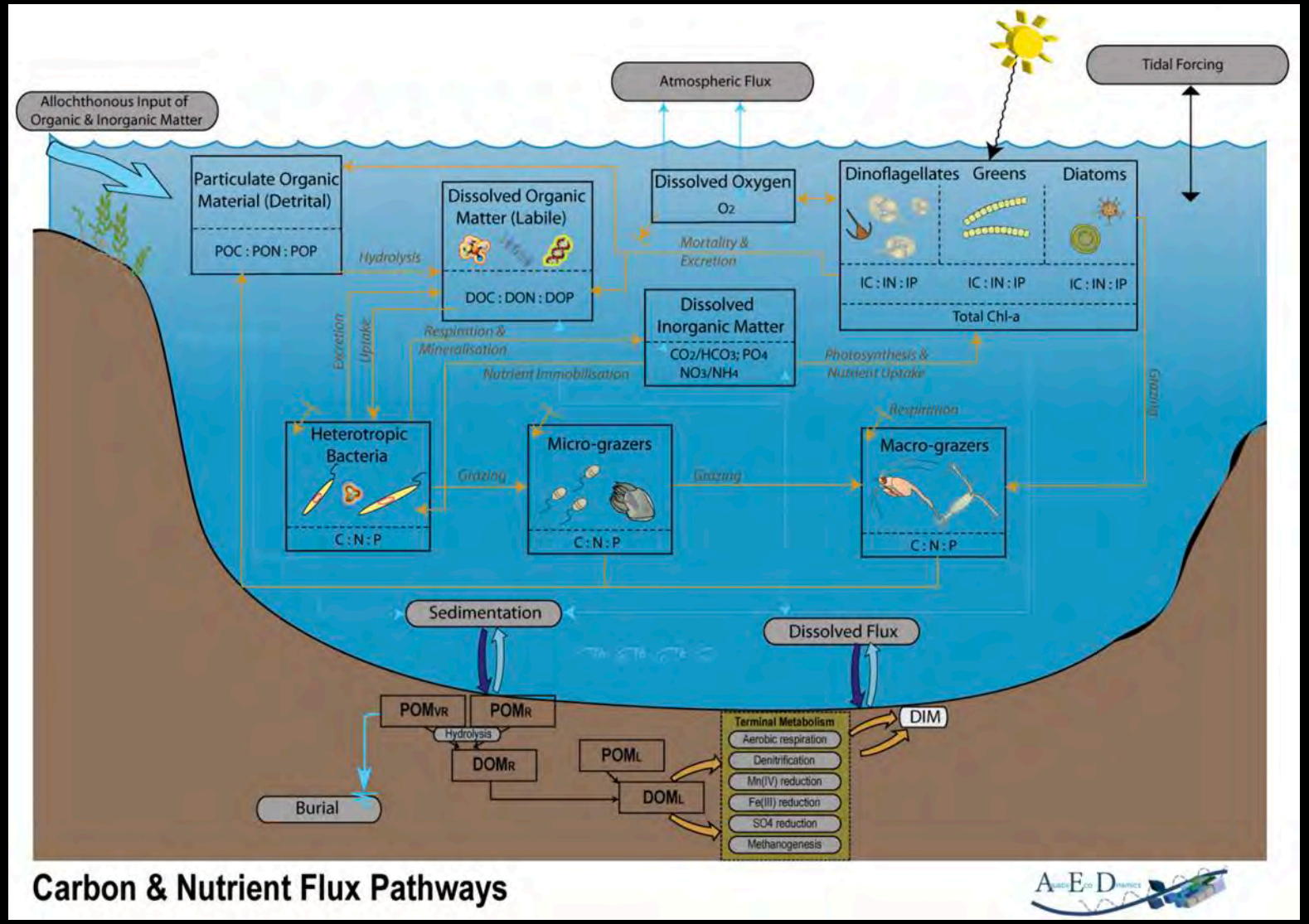
Introduction to GLM

- 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



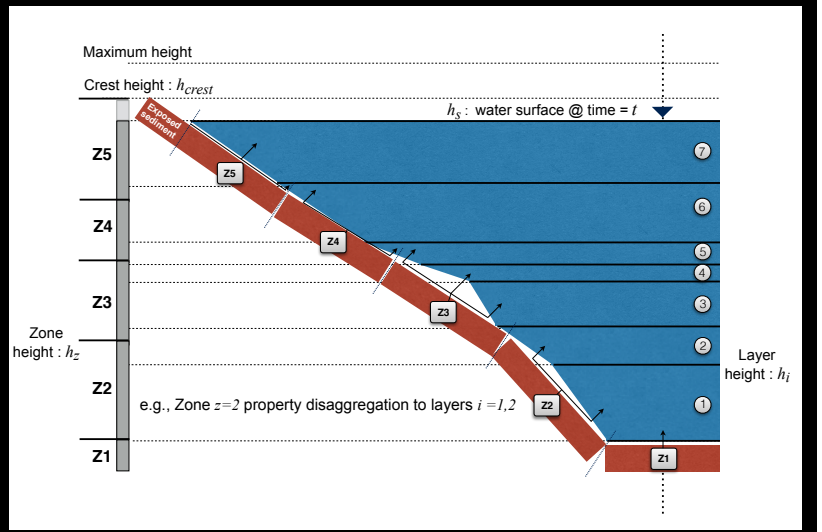
Sneak peek: Water Quality

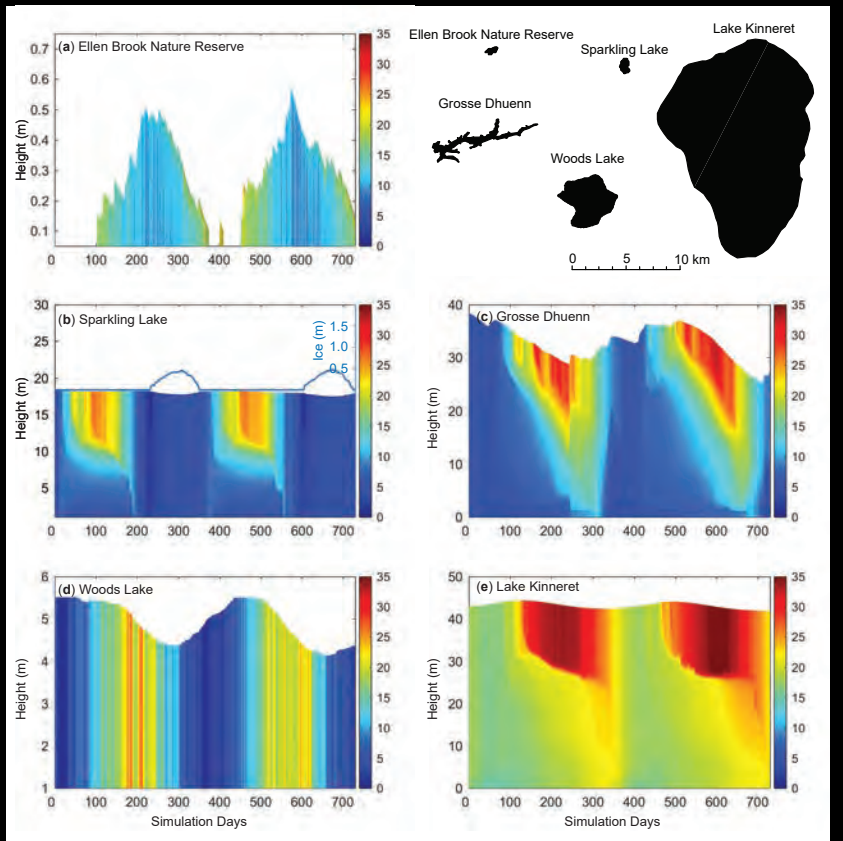
- Aquatic Ecosystem Modelling Library (**AED2**)
- Consists of several modules to conceptualize individual ecosystems, eg:
  - oxygen, nitrogen, phosphorus, phytoplankton
  - sediment biogeochemistry
  - benthic communities
- GLM was designed to interact with AED2



New features in v.3.X

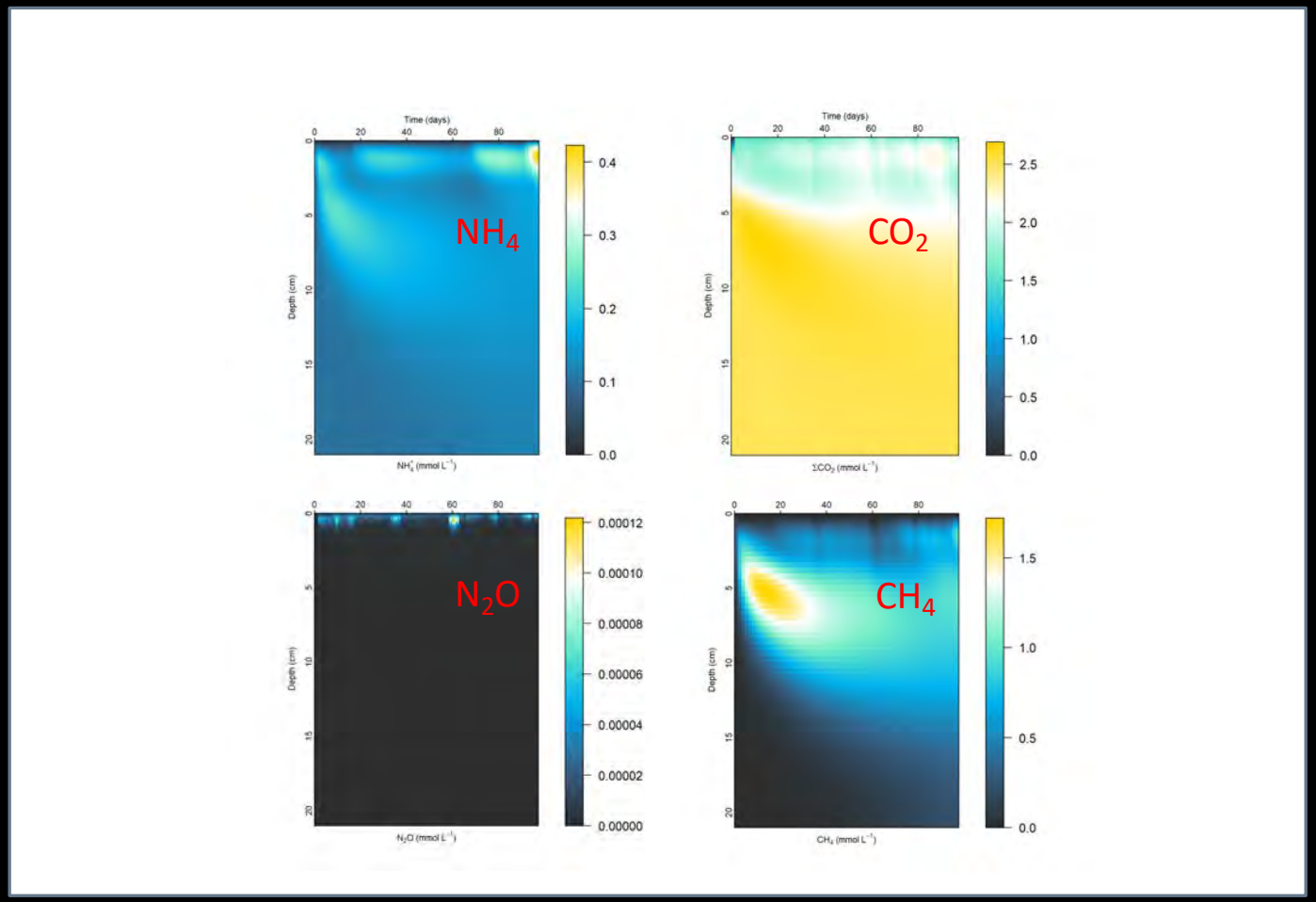
- Sediment-depth zones and zone-specific sediment heating, and biogeochemistry
- Shallow lakes, ponds & wetland simulations (incl. drying out)
- Wind-sheltering options
- Seepage model
- Ice initialization
- Light model





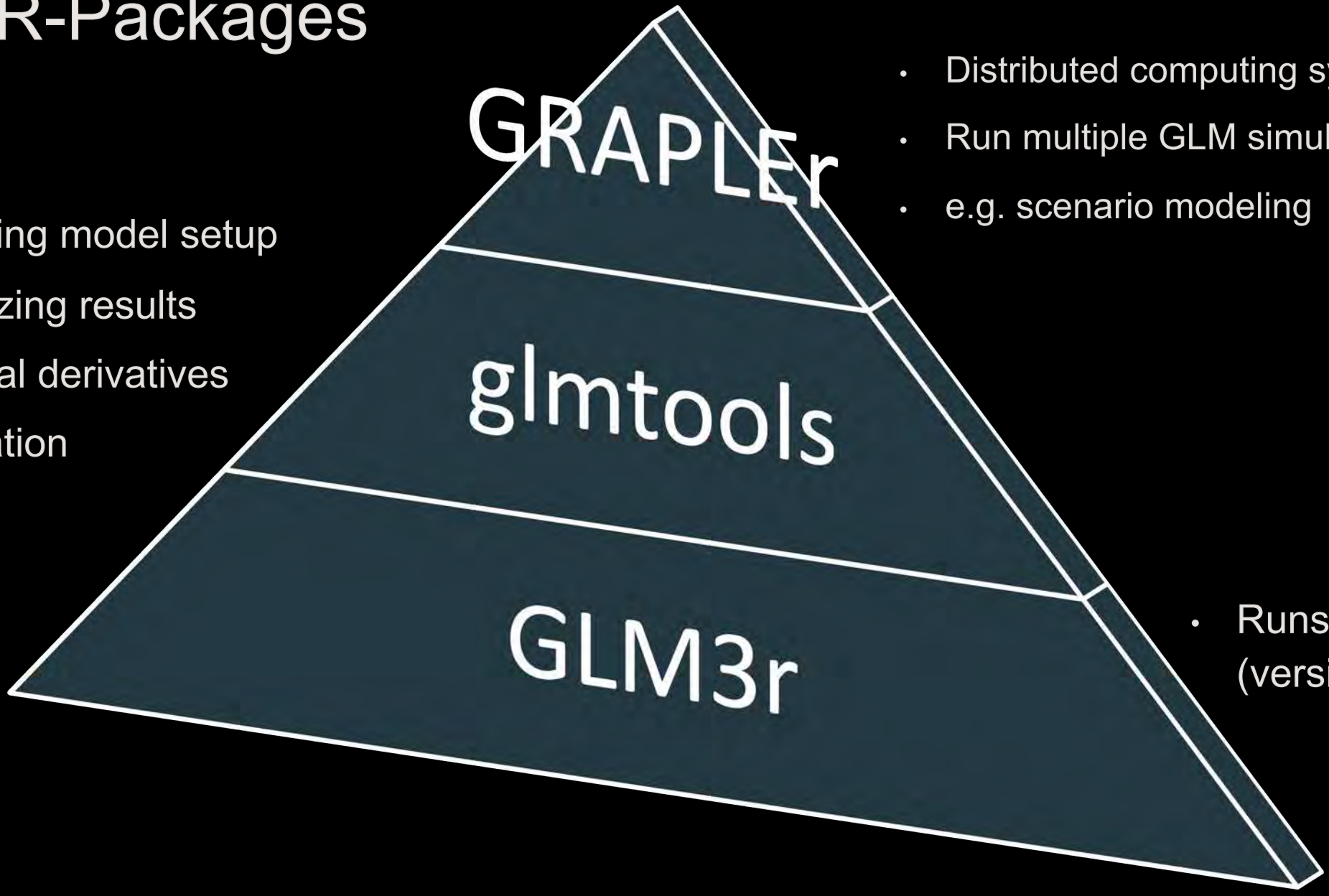
New features in v.3.X

- Water Quality updates (AED2 / AED2+) :
  - GHGs (N2O, CH4, CO2)
  - Benthic productivity (MPB, MAC, MAG)
  - Mussels (BIV)
  - Geochemistry (GEO)
  - Sediment diagenesis (SDG)



GLM R-Packages

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



- Distributed computing system
- Run multiple GLM simulations
- e.g. scenario modeling

- Runs GLM in R (version 3.0.5)

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

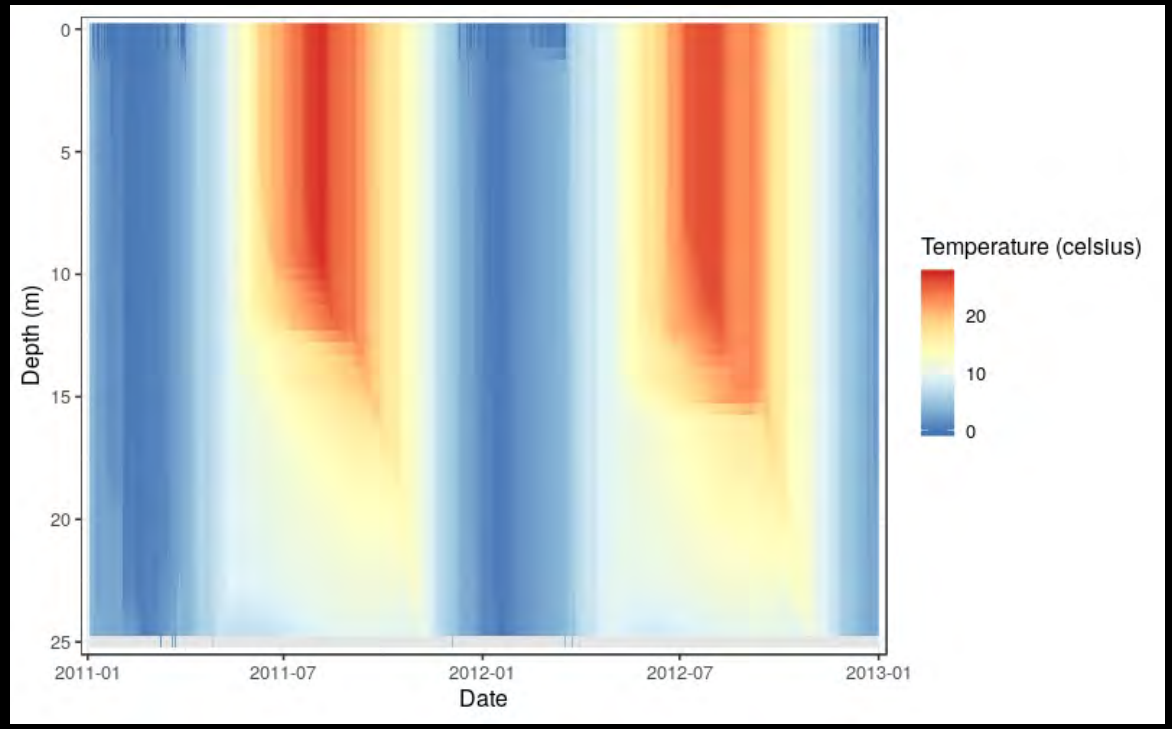
Run

```
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**




Run GLM in R

Break

glmtools: calibration

Template: your specific lake file

glm4.nml

`get_calib_periods()`: calibration

`get_calib_setup()`: variables

glm3.nml

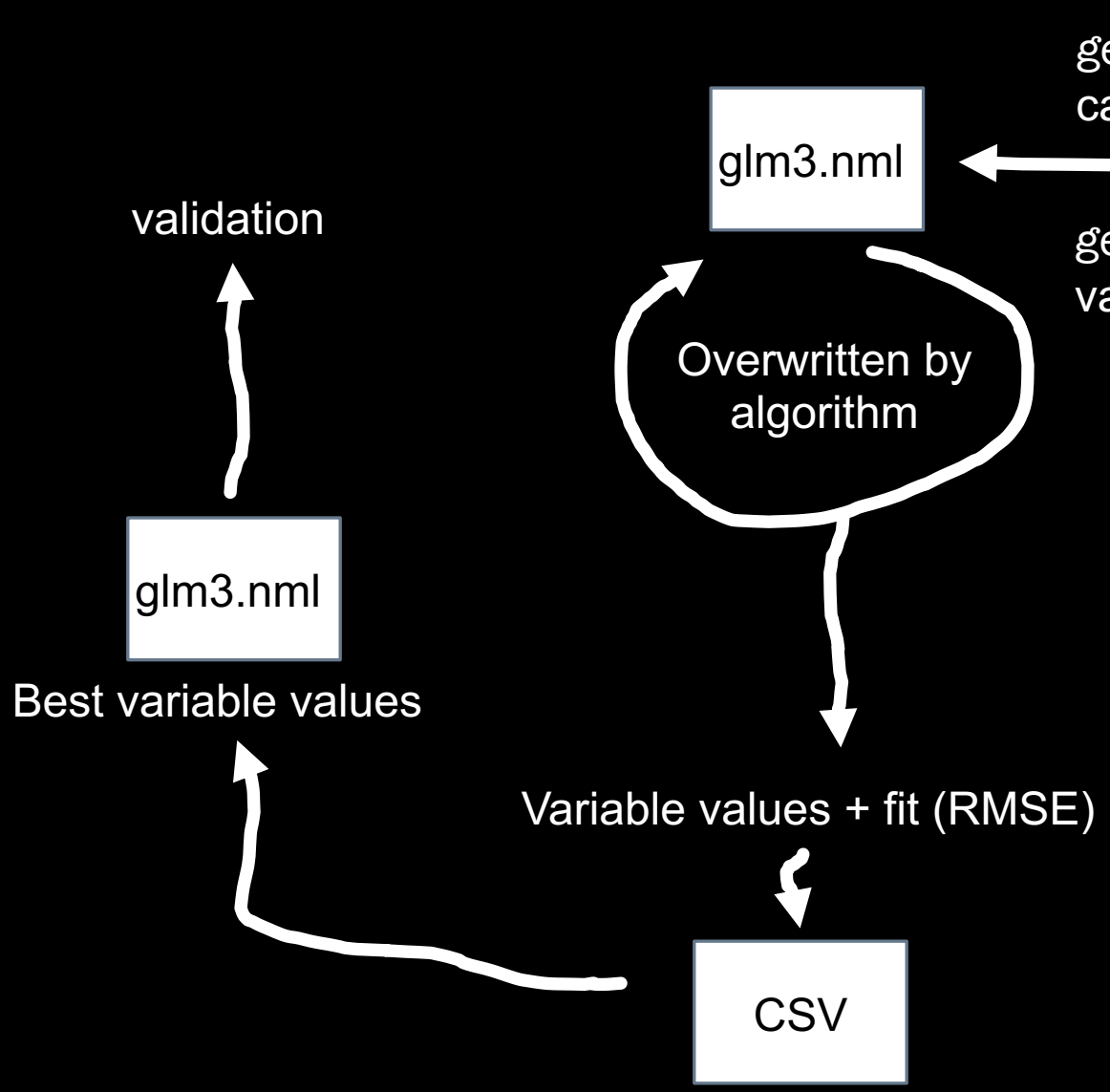
	parameter	lower boundary	upper boundary	initial guess
	pars	lb	ub	x0
1	wind_factor	0.7	2.0	1.0
2	lw_factor	0.7	2.0	1.0
3	Kw	0.1	0.8	0.5
4	sed_temp_mean	3.0	8.0	5.0
5	sed_temp_mean	8.0	20.0	15.0

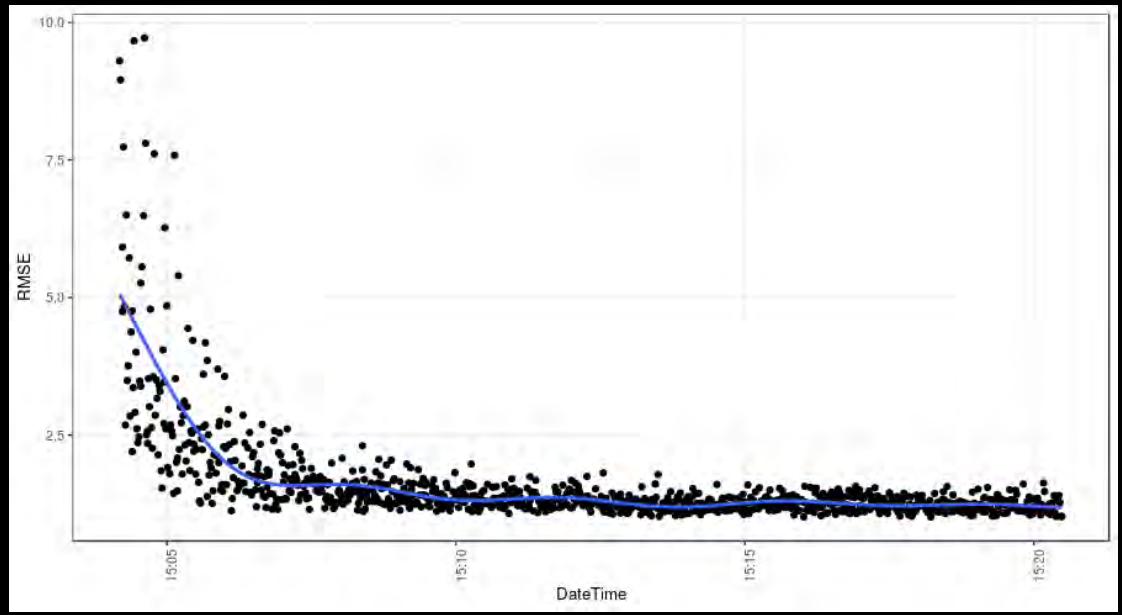
Identified as sensitive by global lake modeling project ISIMIP

Sediment heat mean temperatures to improve vertical water temperature fit

ISIMIP
Inter-Sectoral Impact Model Intercomparison Project

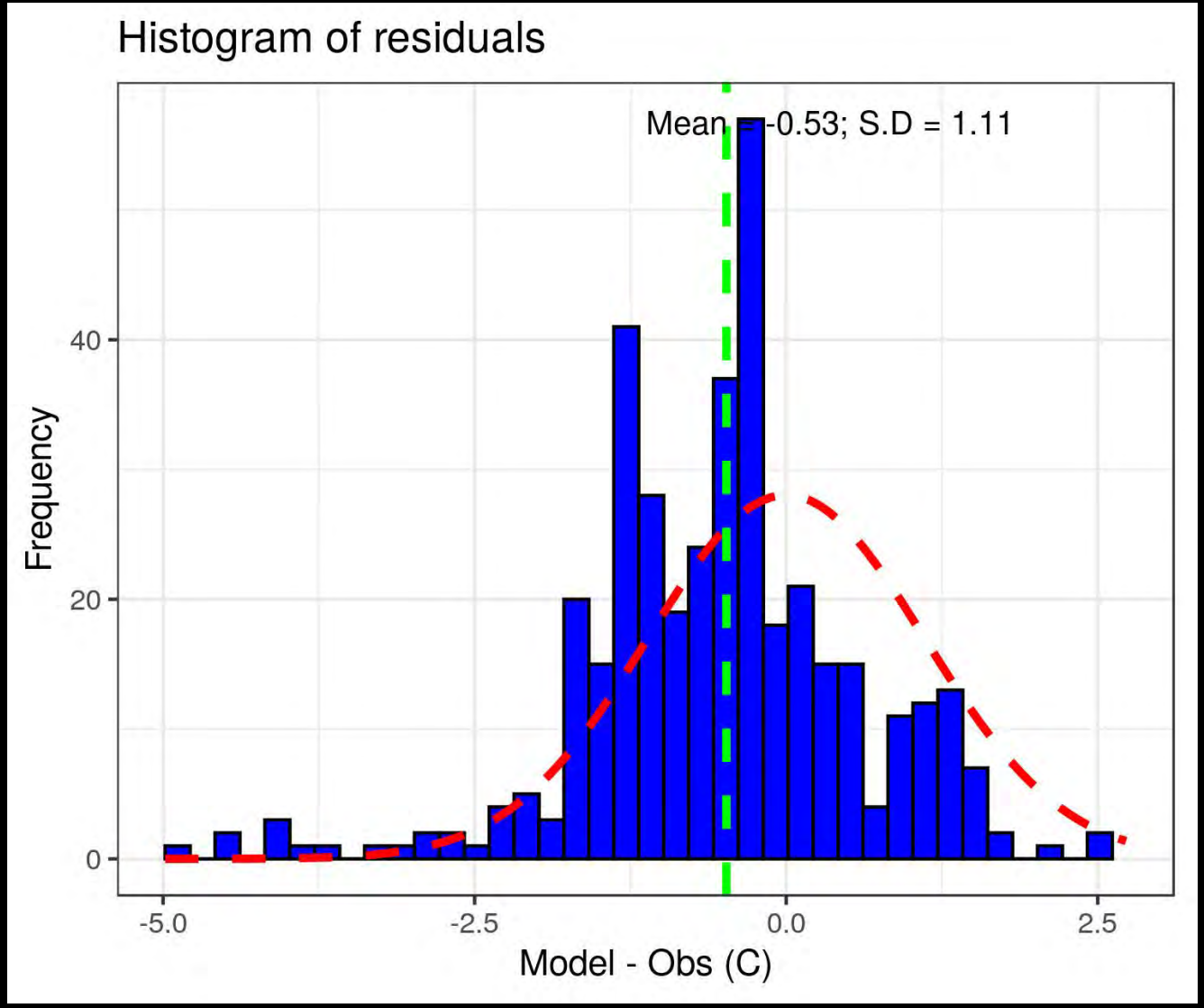
glmtools: calibration





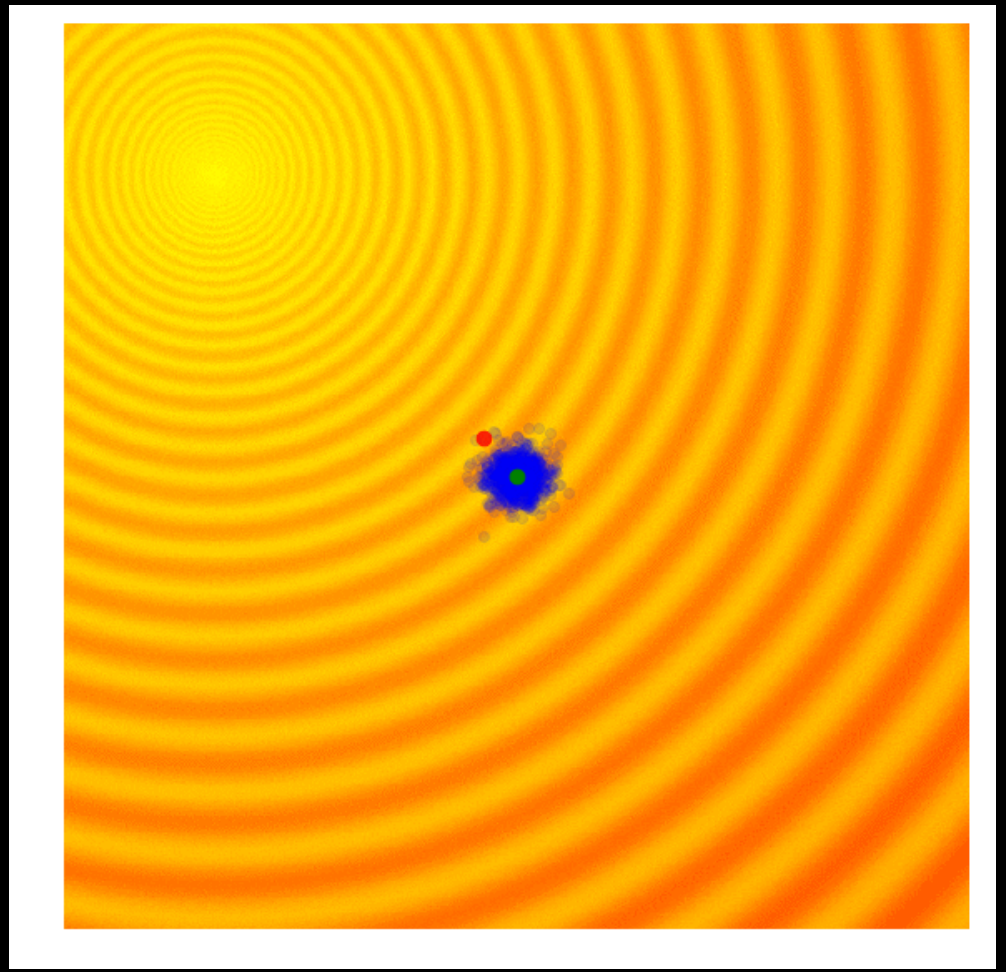
glmtools: calibration

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

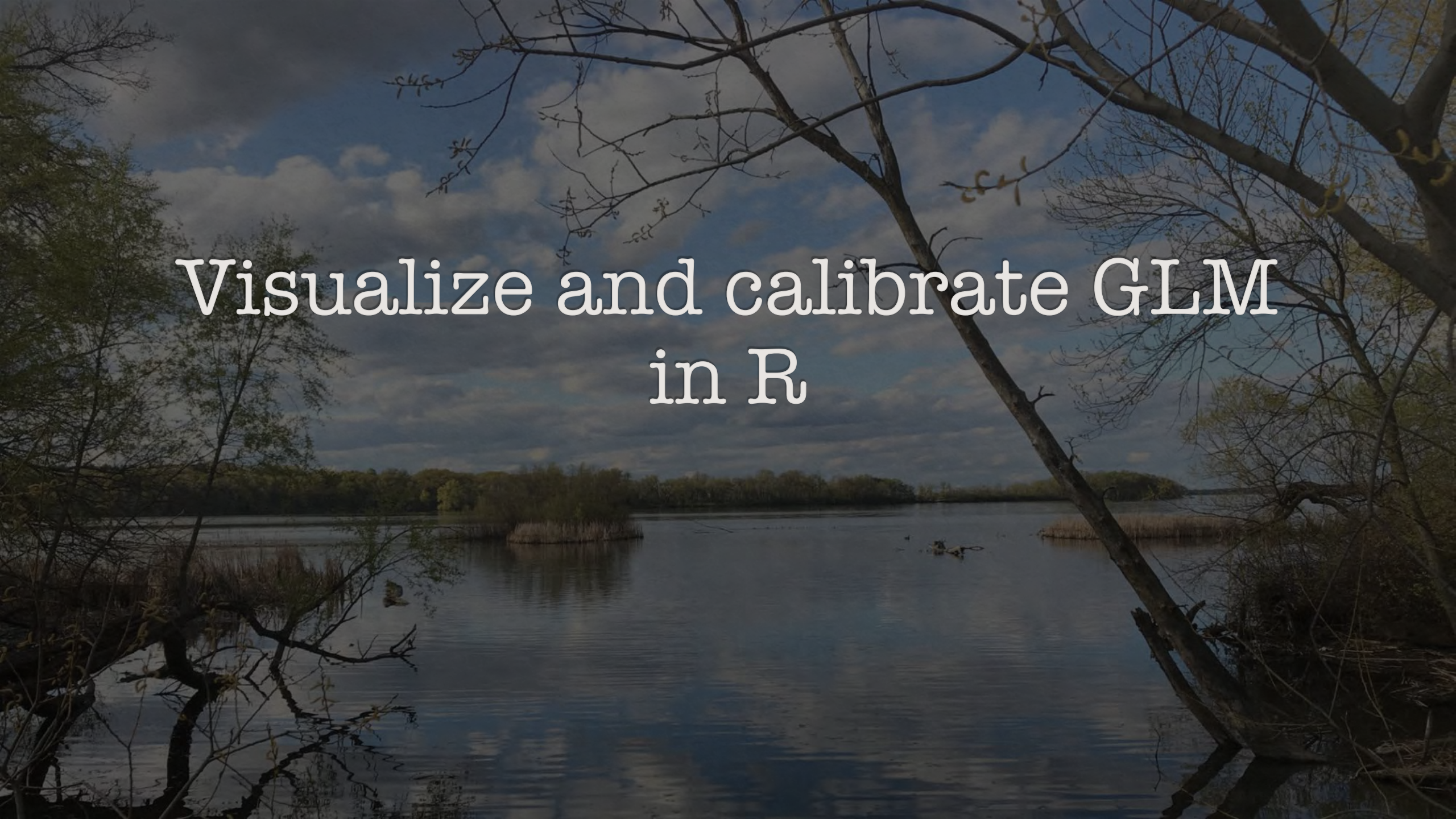


Evolutionary optimization (default)

- 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 ℃) or doing a finite amount of iterations (default is 150)

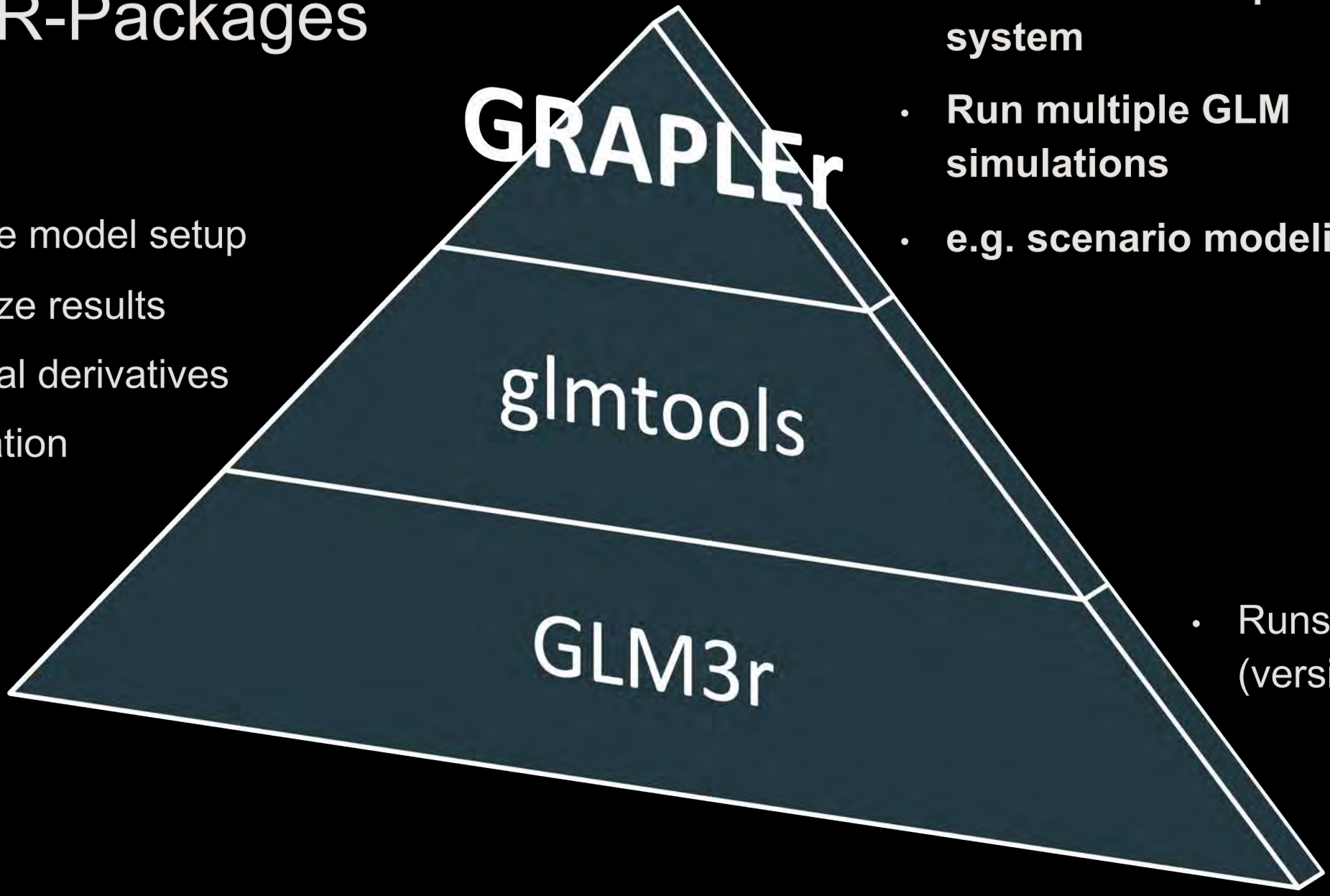


Visual example (link)


Visualize and calibrate GLM
in R

GLM R-Packages

- Change model setup
- Visualize results
- Physical derivatives
- Calibration



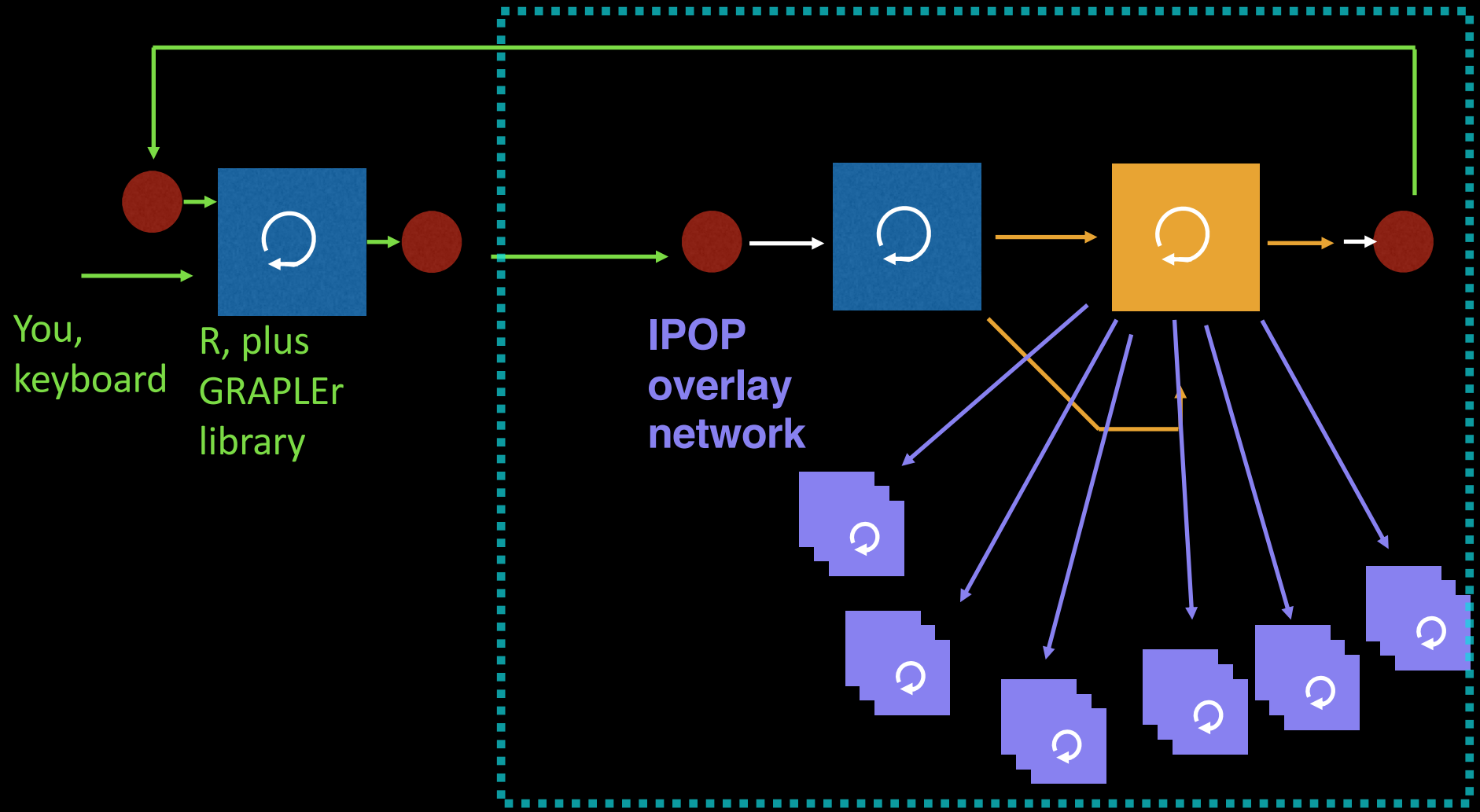
- **Distributed computing system**
- **Run multiple GLM simulations**
- **e.g. scenario modeling**

- Runs GLM in R (version 3.0.5)

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

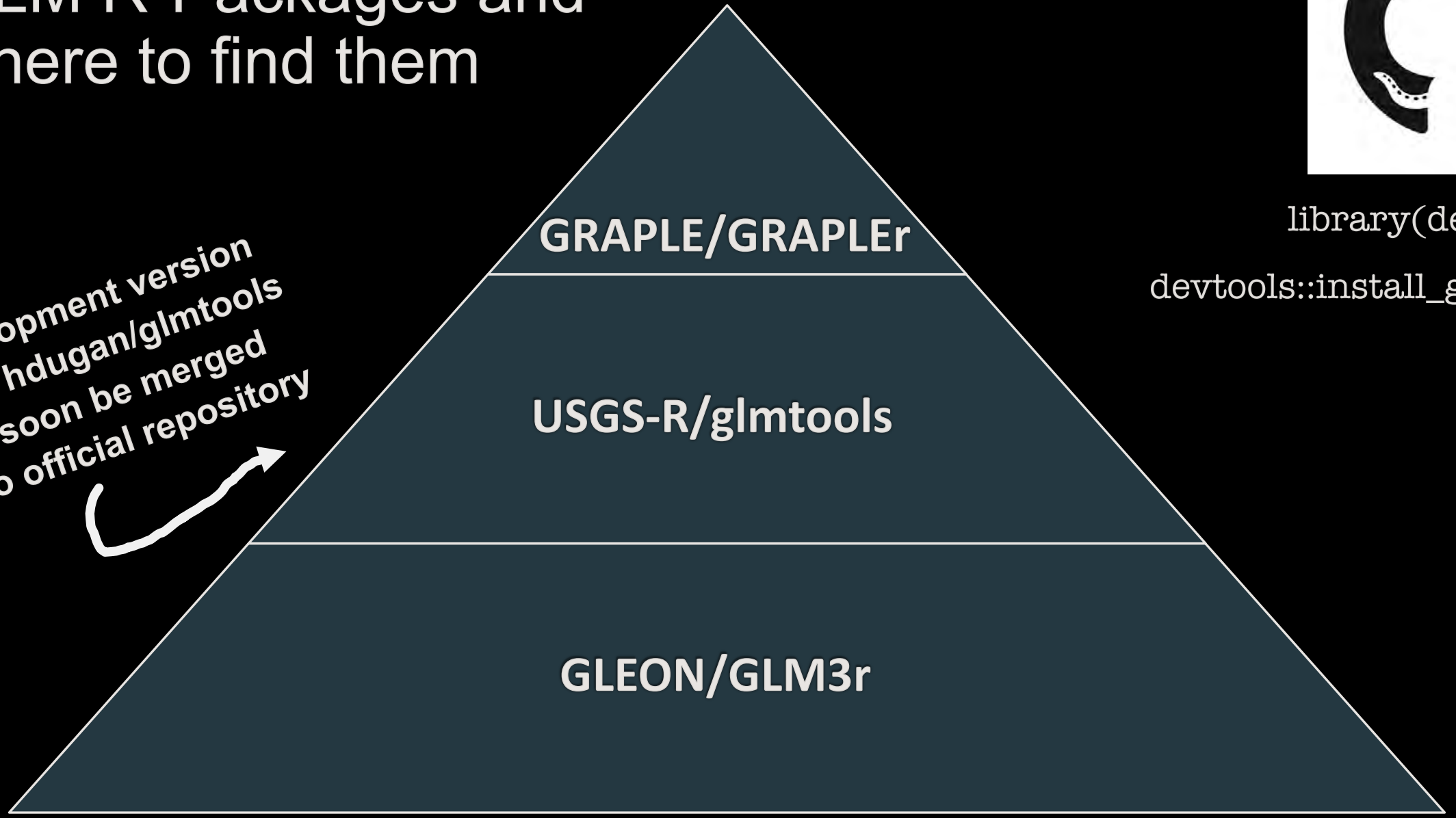
GRAPLEr under the hood



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

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!

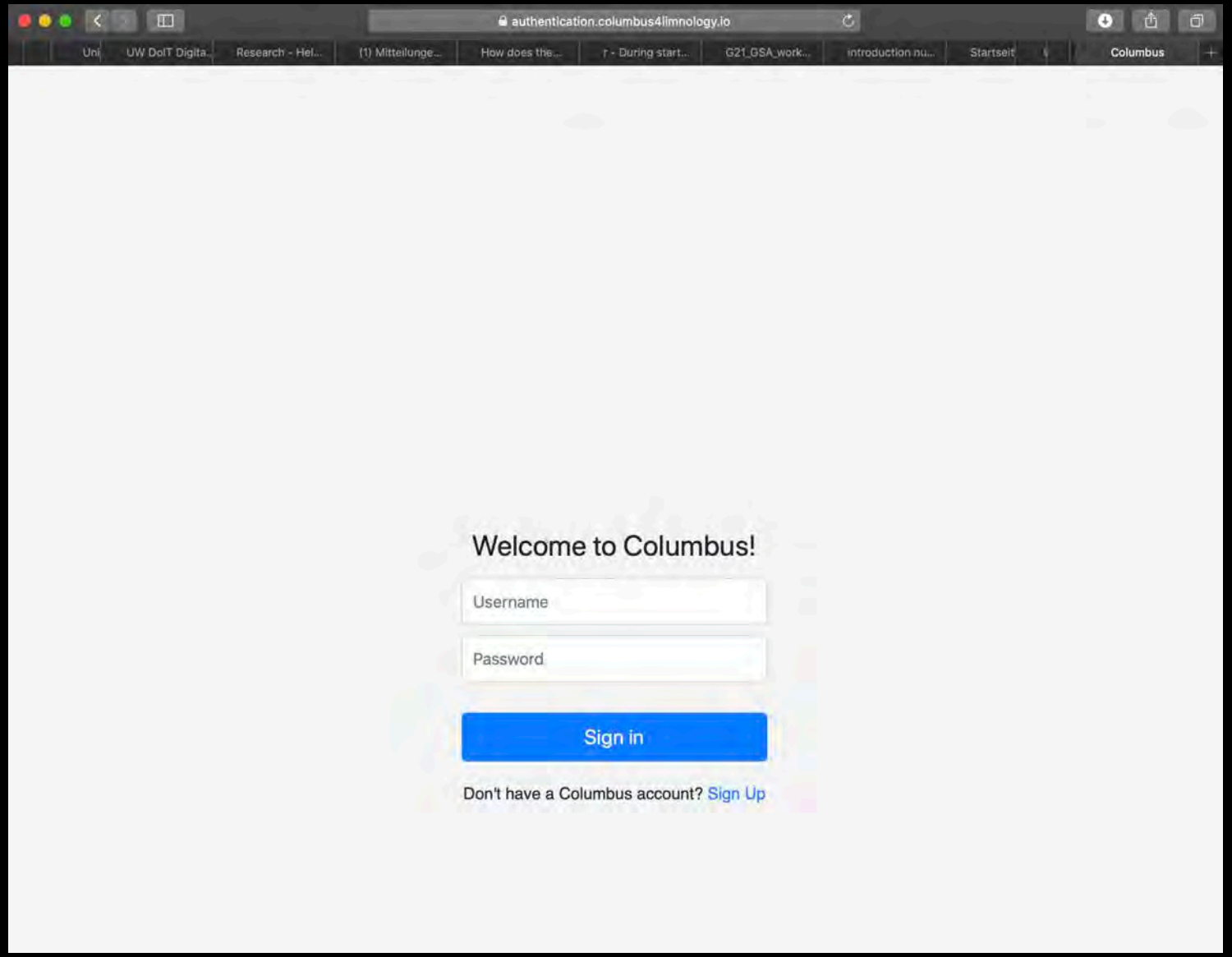
Demonstration

AnHai Doan
Prof. @ CS
UW-Madison

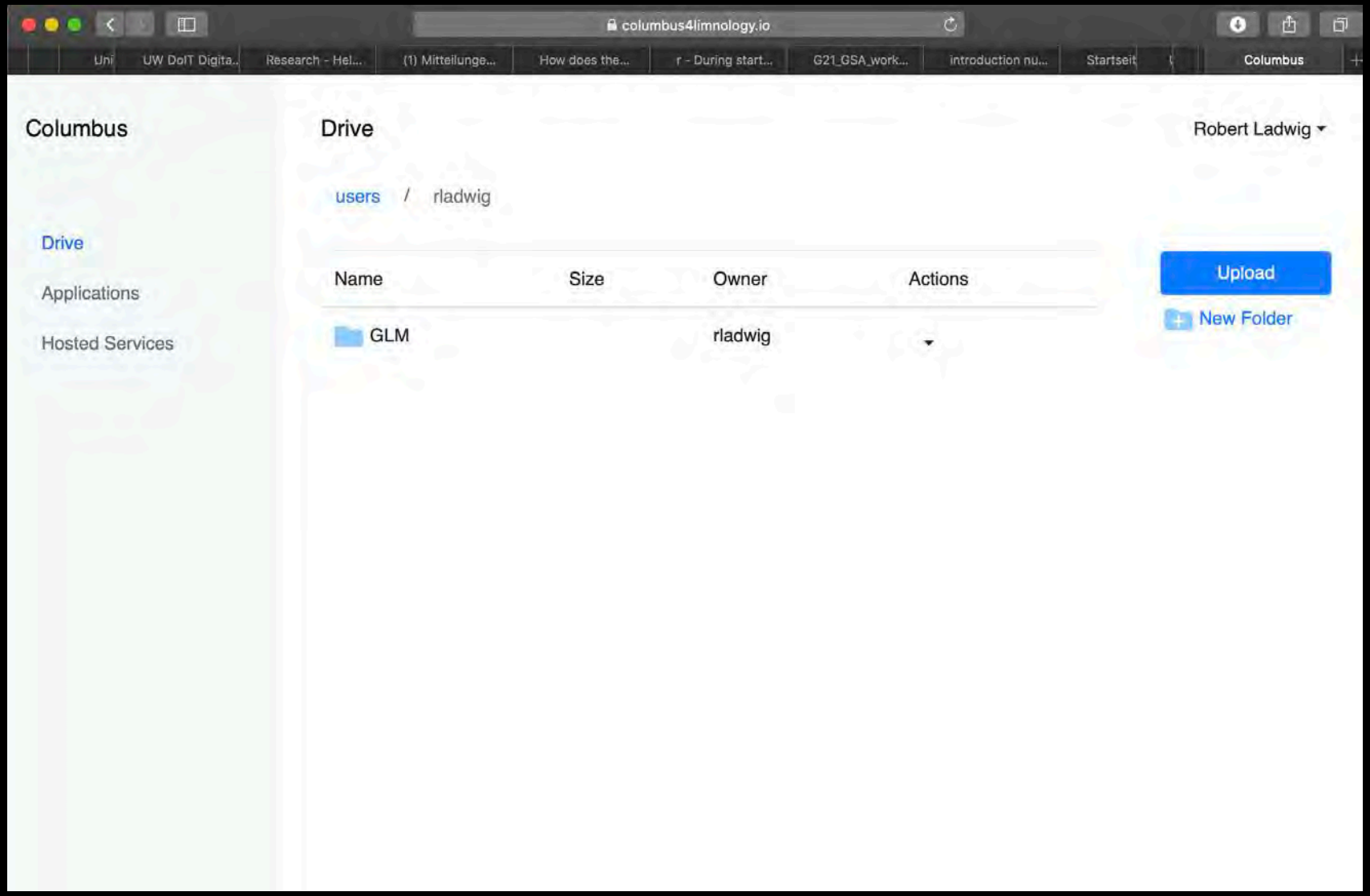
columbus4limnology.io

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

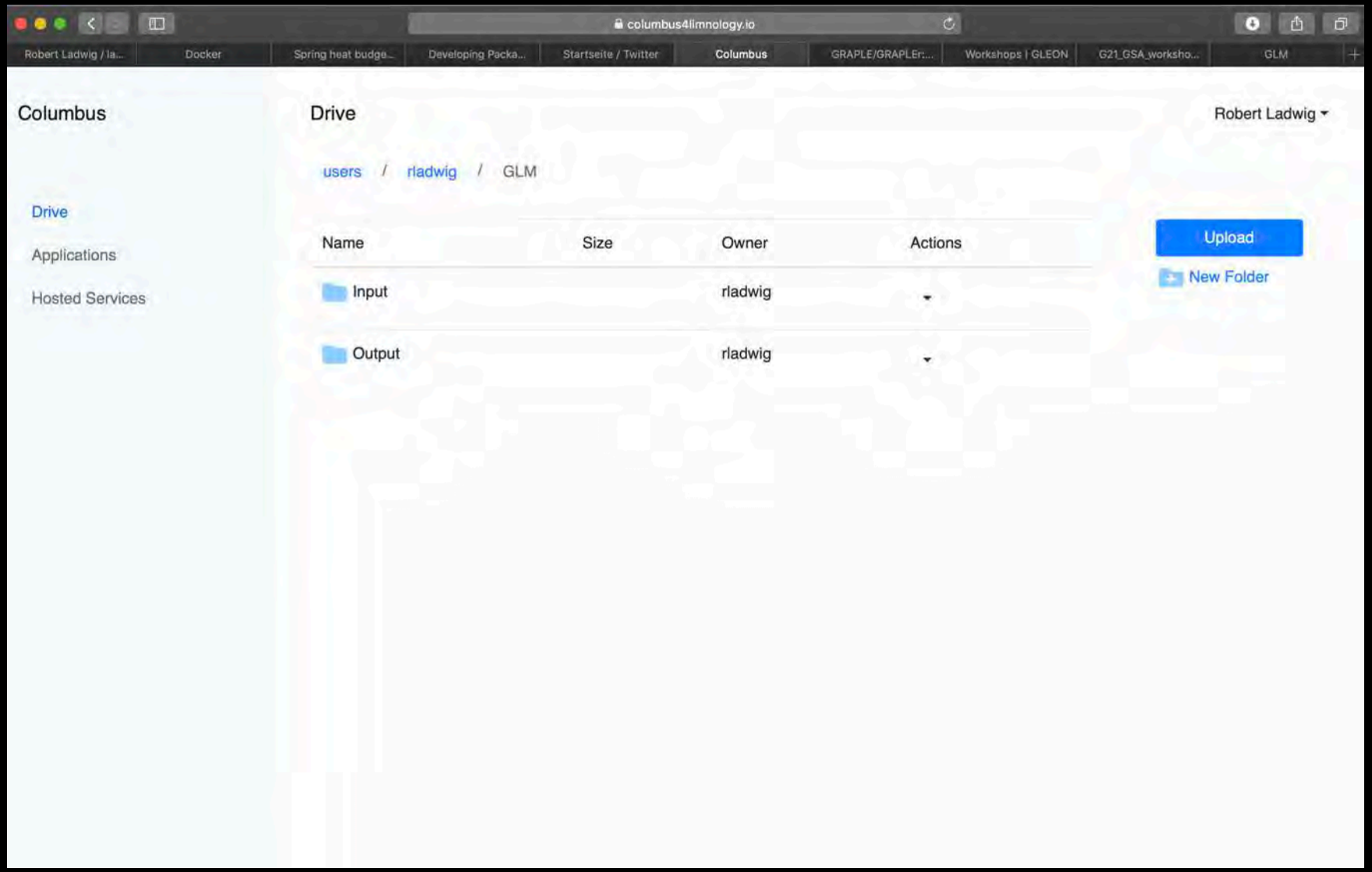
Create an account



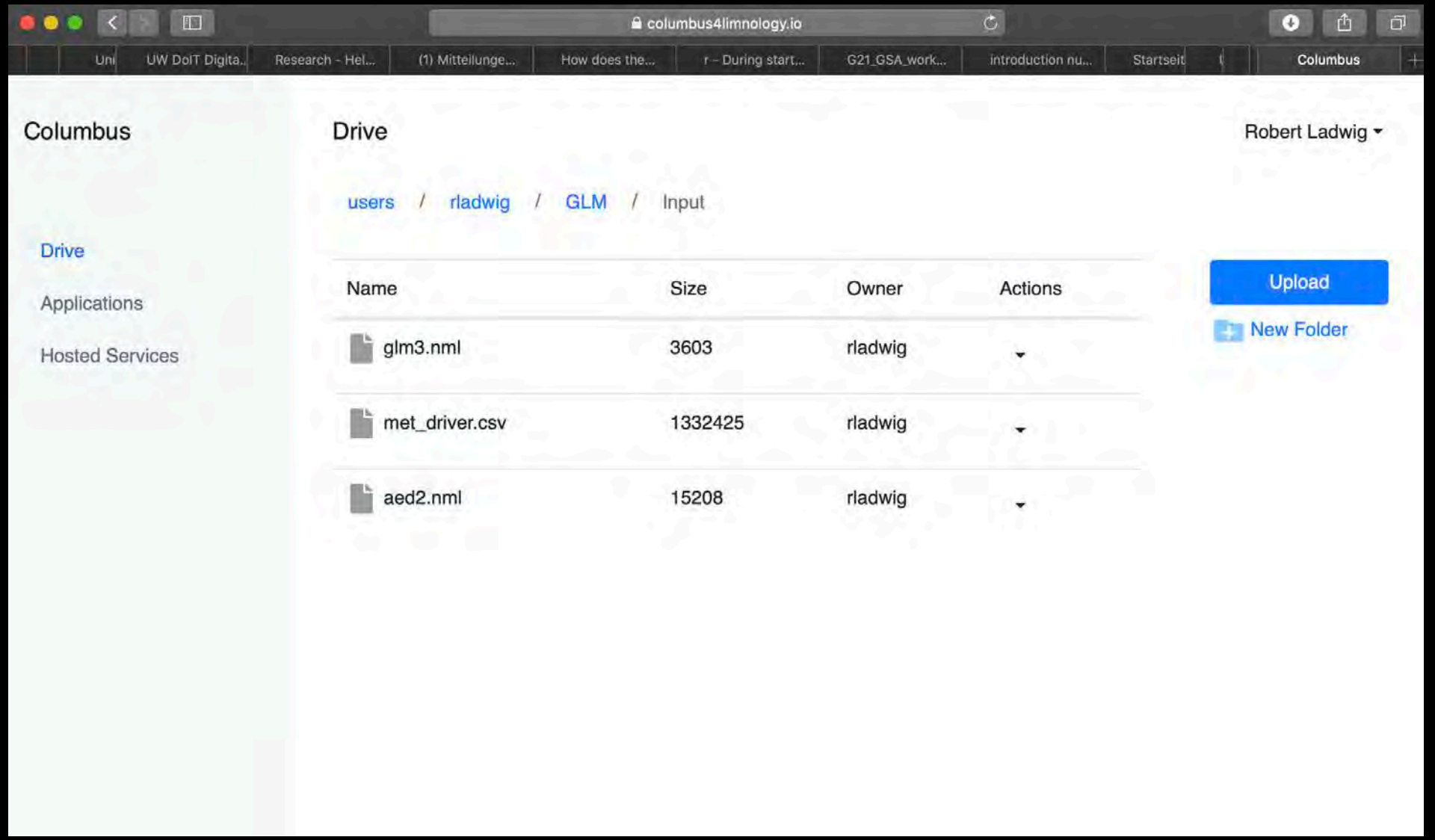
Upload your model setup



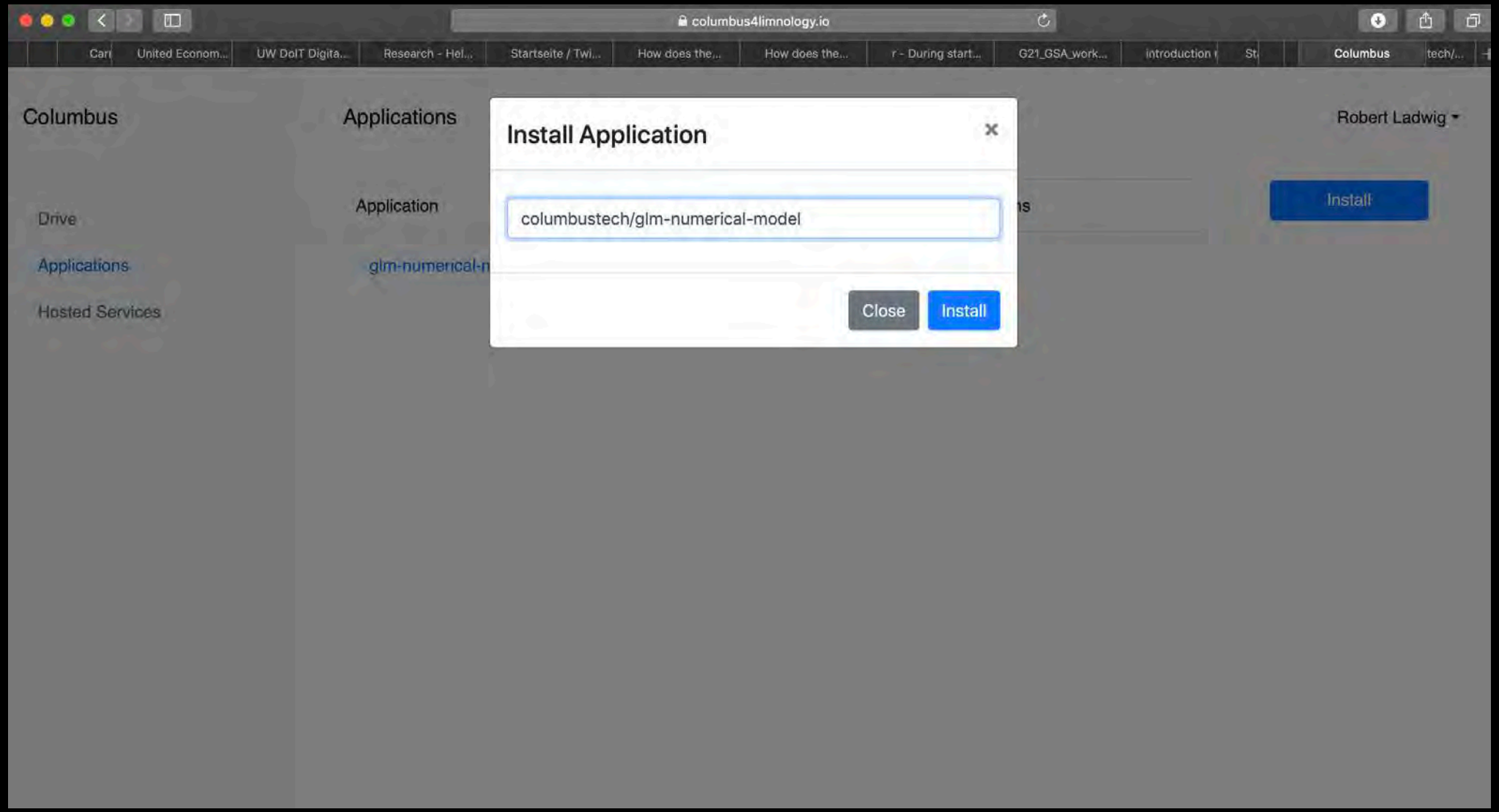
Have two folders



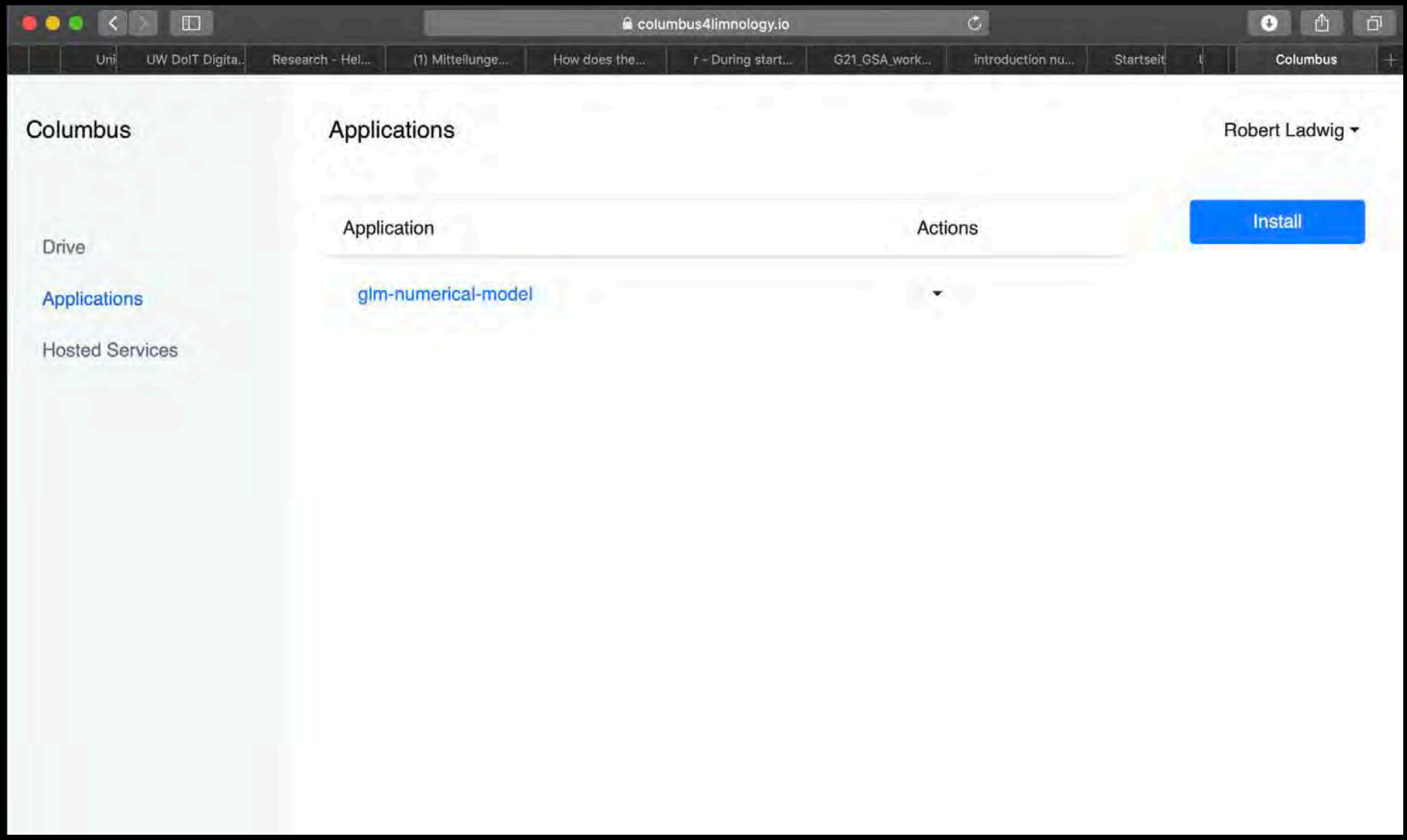
You'll need a glm3.nml file and driver data



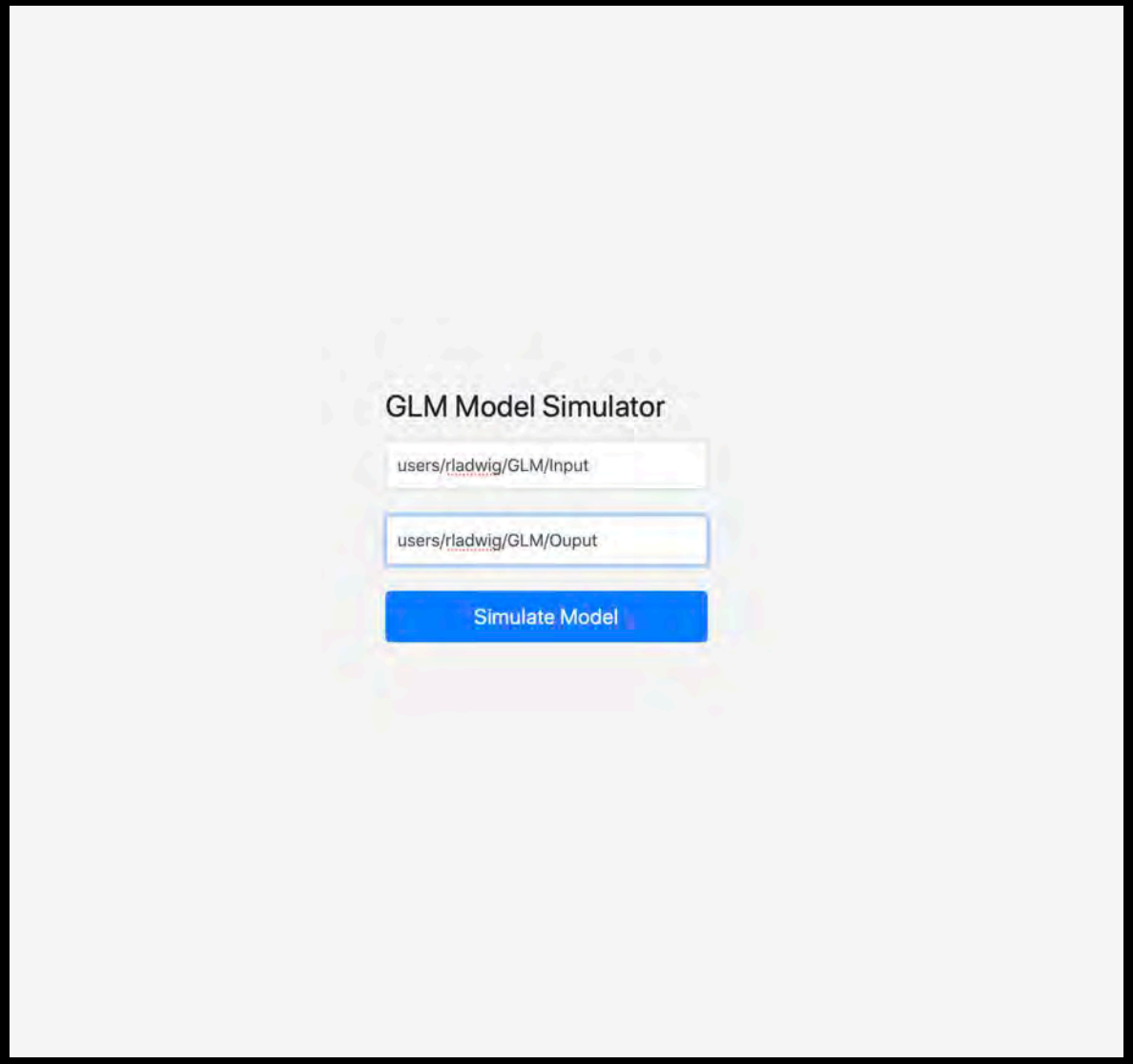
Install the docker container



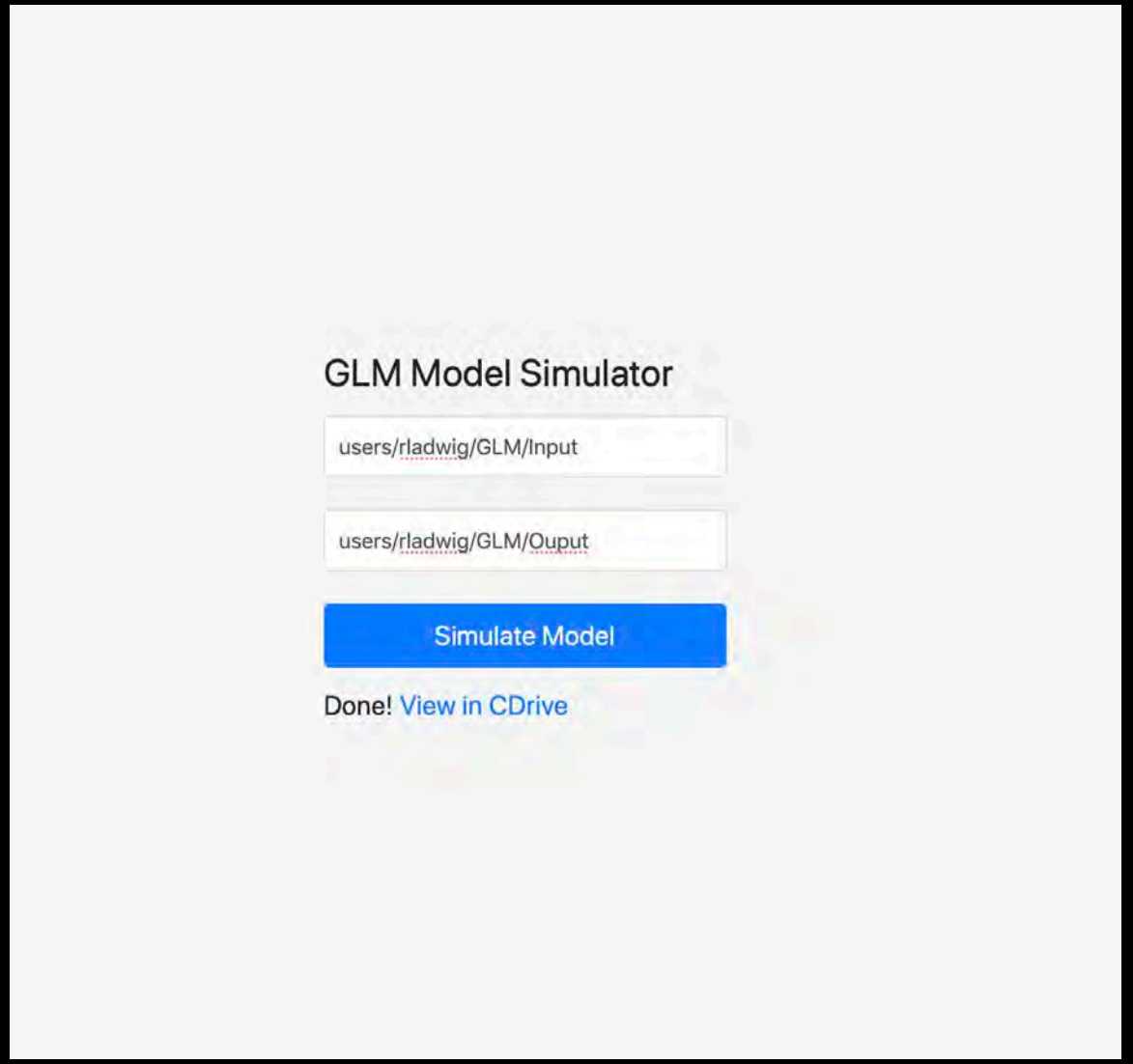
Click on the application



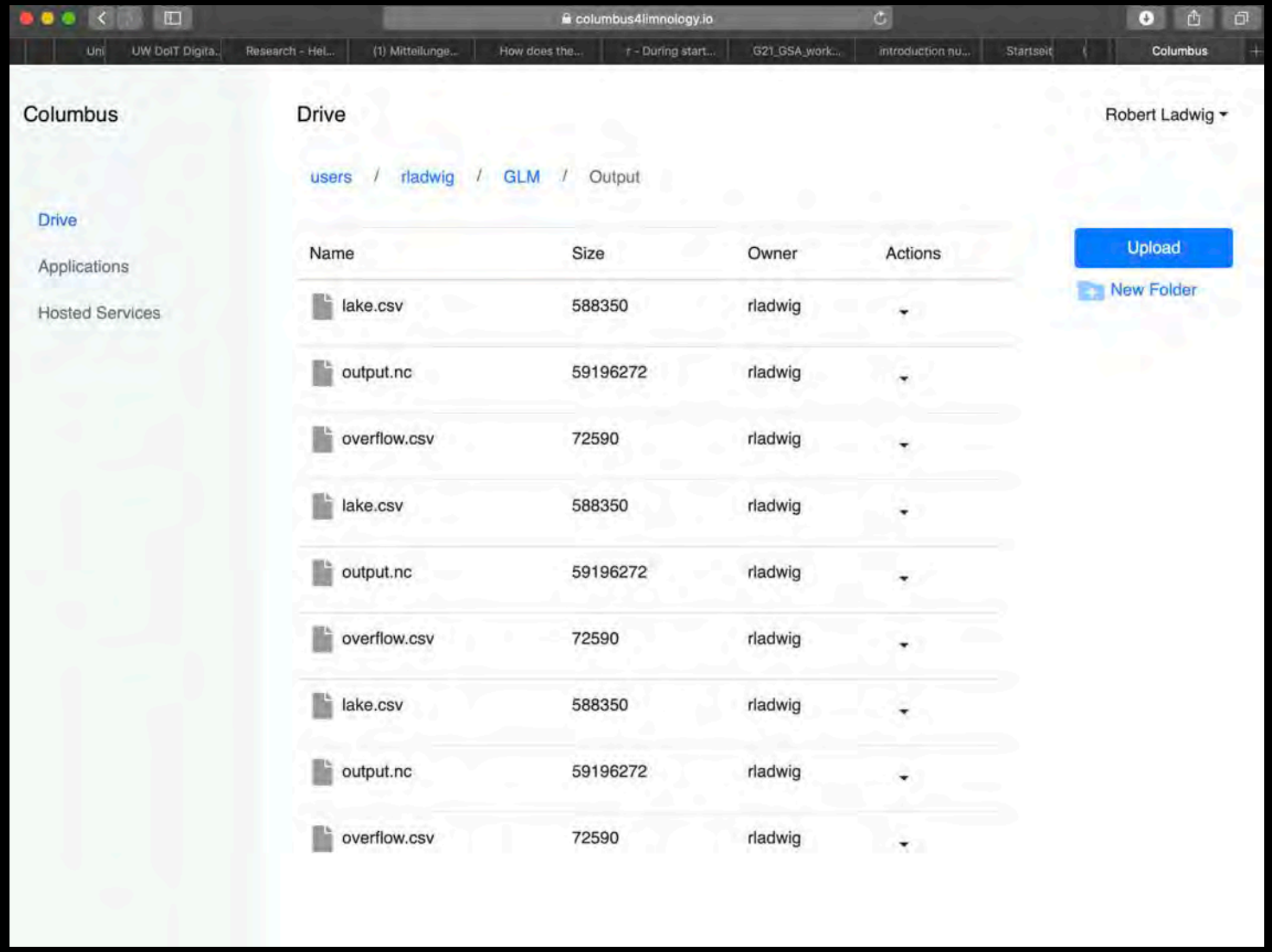
Type in the input and output paths



Simulate model



Download the output



columbus4limnology.io

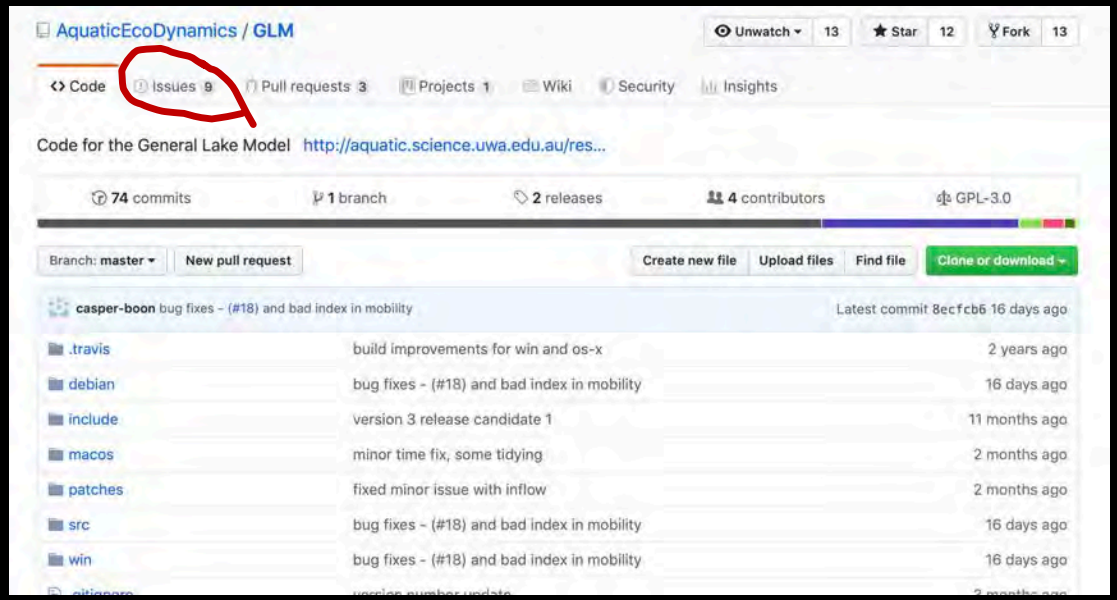
- Feel free to create an account and to run GLM simulations in the cloud!

- 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

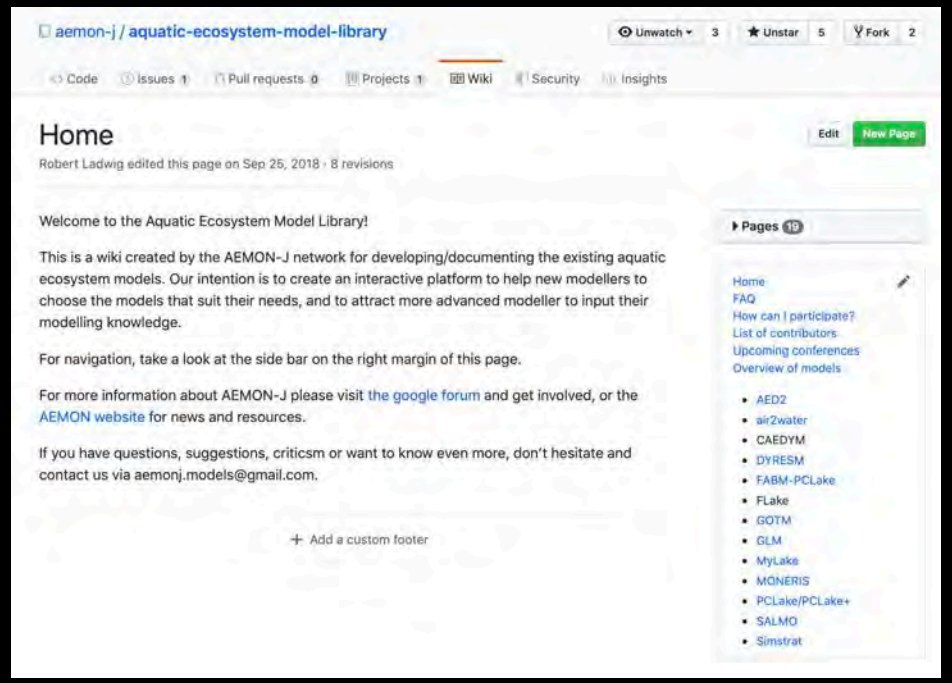
- Find latest source code at https://github.com/AquaticEcoDynamics/GLM
- Here, you can raise issues (errors, compilation problems, suggestions, improvements, bugs)



- 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



Next AEMON J 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/AquaticEcoDynamics/GLM
- Here, you can raise issues (errors, compilation problems, suggestions, improvements, bugs)

- Join GLM slack to ask questions and get