

# PRAGMA-GLEON Expedition (GRAPLE) - Lake Science on Overlay-networked Resources

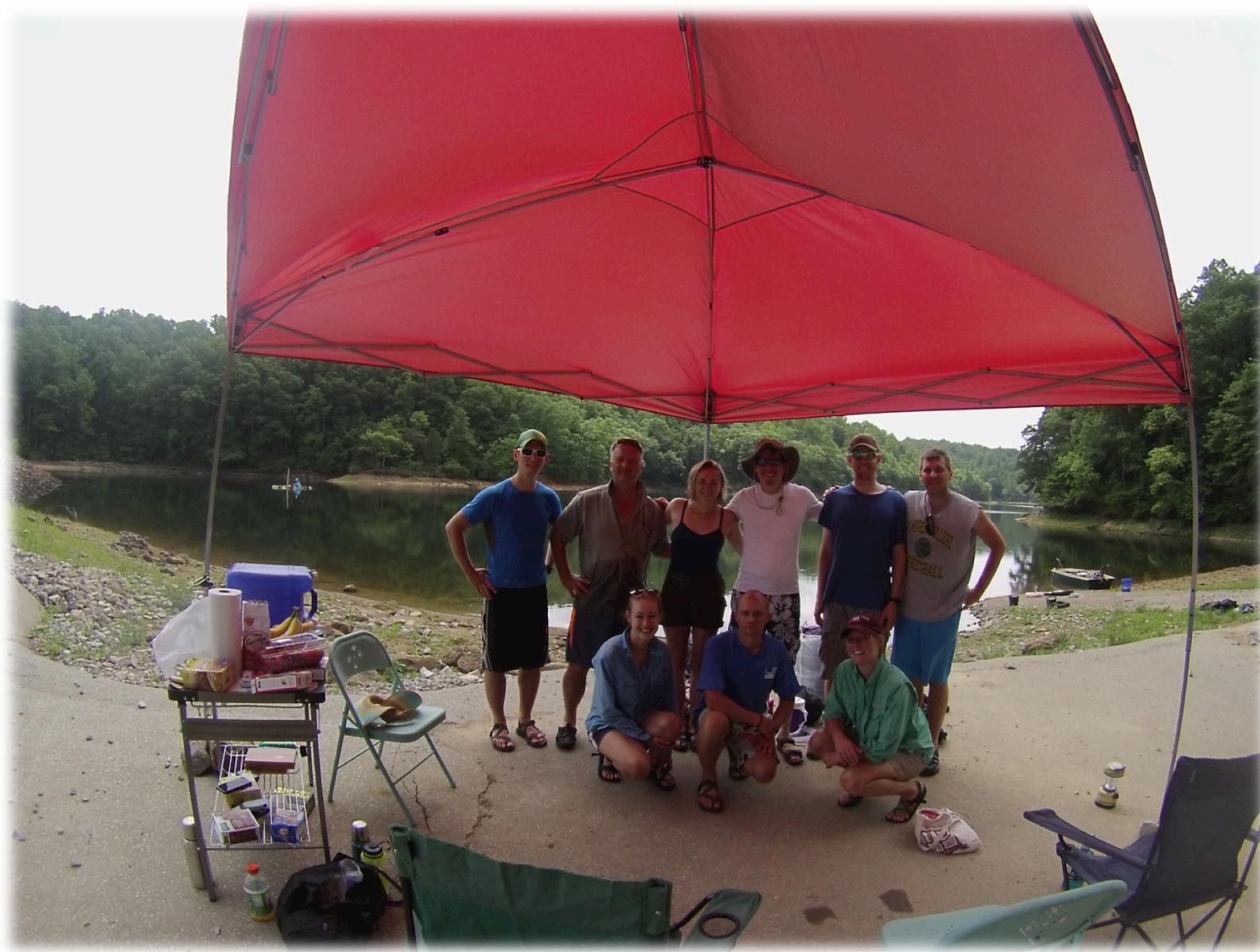
Paul Hanson (University of Wisconsin)

Cayelan Carey (Virginia Tech)

Renato Figueiredo, Ken Subratie, Saumitra Aditya  
(University of Florida)

# Ecologists in their natural environment

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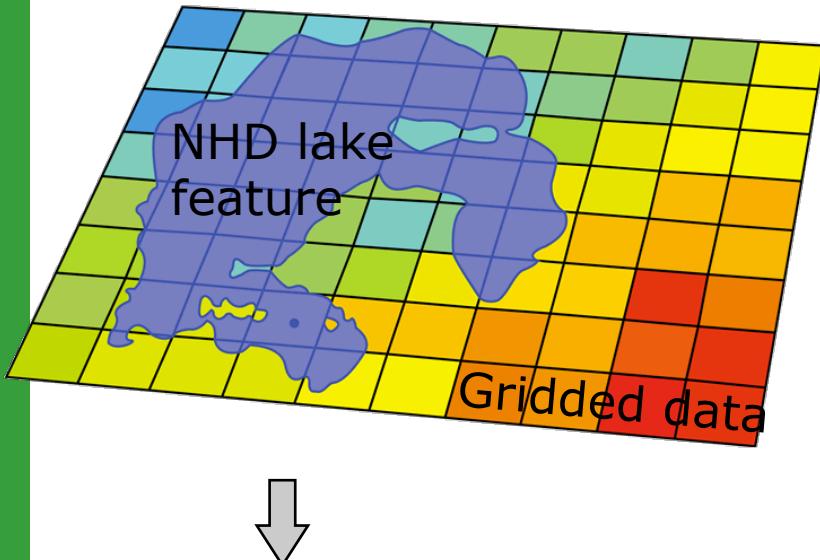
# Questions like this...

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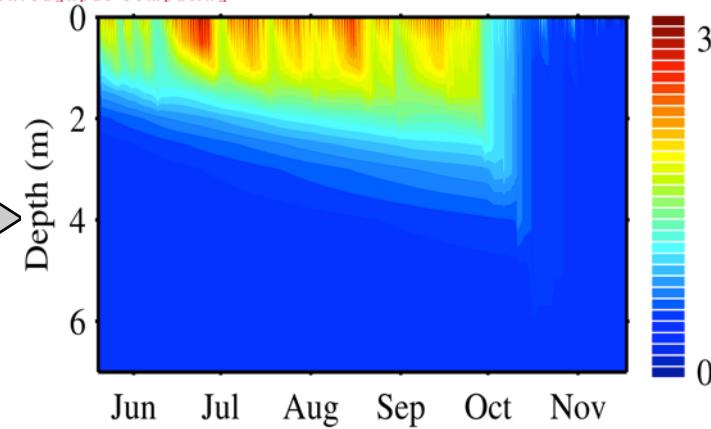
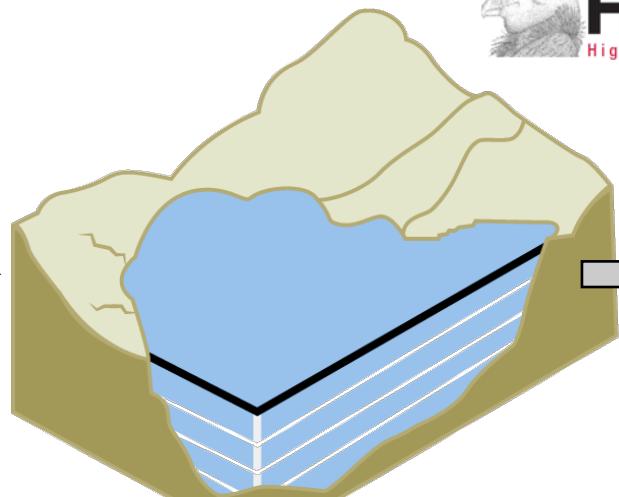
*How will the availability and quality of water respond to changes in land use and climate?*

Often require...

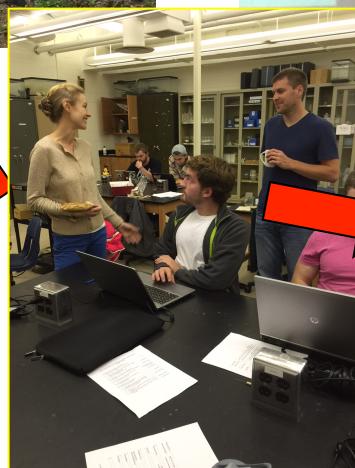
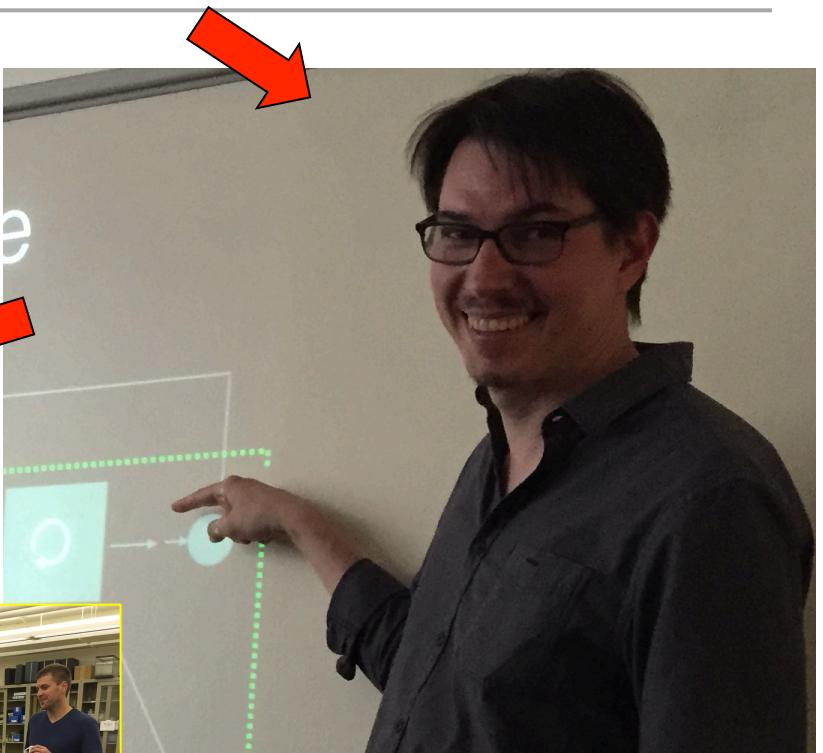
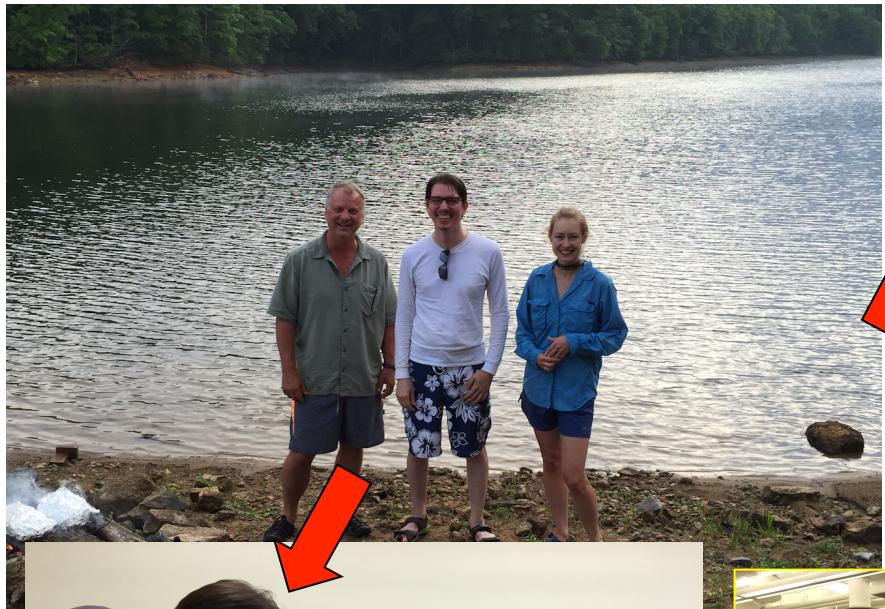
...approaches like this.



- Parameterization of models with gridded data
- Dynamic lake temperature simulations
  - Parallel computing with



# Our solution?



# Landscape of numerical simulation

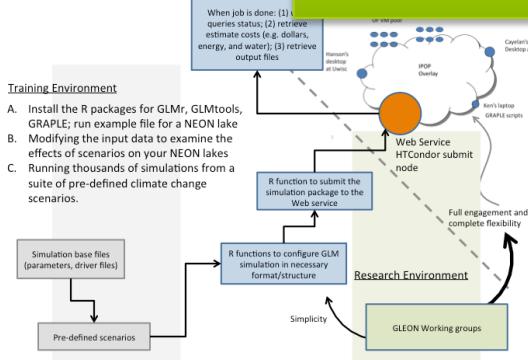
UWA

Matt Hipsey

PRAGMA

Simulation software development

Compute infrastructure



GitHub

USGS-CIDA  
Jordan Read  
Luke Winslow

R-based GLM tools

Papers, sample parameter sets

Training & education

User community  
Waikato U. (NZ)  
U. Adelaide (Australia)  
U. Wisconsin (USA)  
Virg. Tech (USA)  
NYC DEP  
Cornell  
USGS  
UWA

## Outcomes of the activities

1. Basic research in science
2. A new kind of science for ecologists
3. Water resource management
4. Education and training (project EDDIE)
5. Data standardization, workflows
6. Community development
7. Cross-discipline training

# Toxic Algae Outbreak Overwhelms a Polluted Ohio River

By MICHAEL WINES SEPT. 30, 2015

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HE NAMED ME  
**MALALA**

The Ohio River, transformed by mining and industrial waste and sewage overflows into the nation's most polluted major waterway, has a new and unexpected tormentor this fall: carpets of poisonous algae.

Pads of toxic blue-green algae have speckled nearly two-thirds of the 981-mile river in the last five weeks, experts say, in an outbreak that has curbed boating, put water utilities on alert and driven the river's few hardy swimmers back to shore.

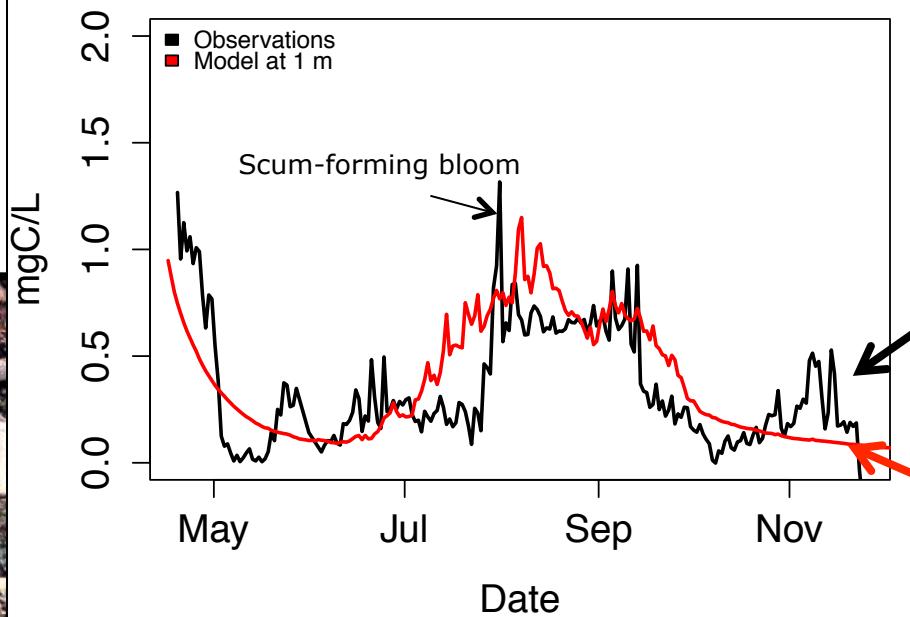
The only other recorded toxic algae bloom, in 2008, covered perhaps 40 miles of the river. In contrast, the latest bloom stretches 636 miles from Wheeling, W.Va., to Cannelton, Ind., and traces of algae have appeared as far west as Illinois.

The poisonous alga, called microcystis,

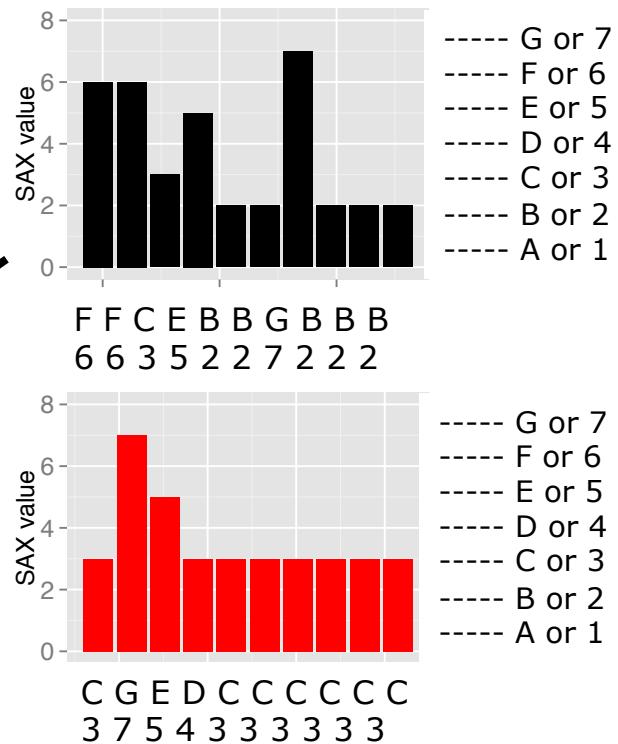


A sample of water with algae from Lake Erie near Curtice, Ohio, in July. The latest bloom of algae stretches along 636 of the Ohio River's 981 miles.  
Eric Albrecht/The Columbus Dispatch, via Associated Press

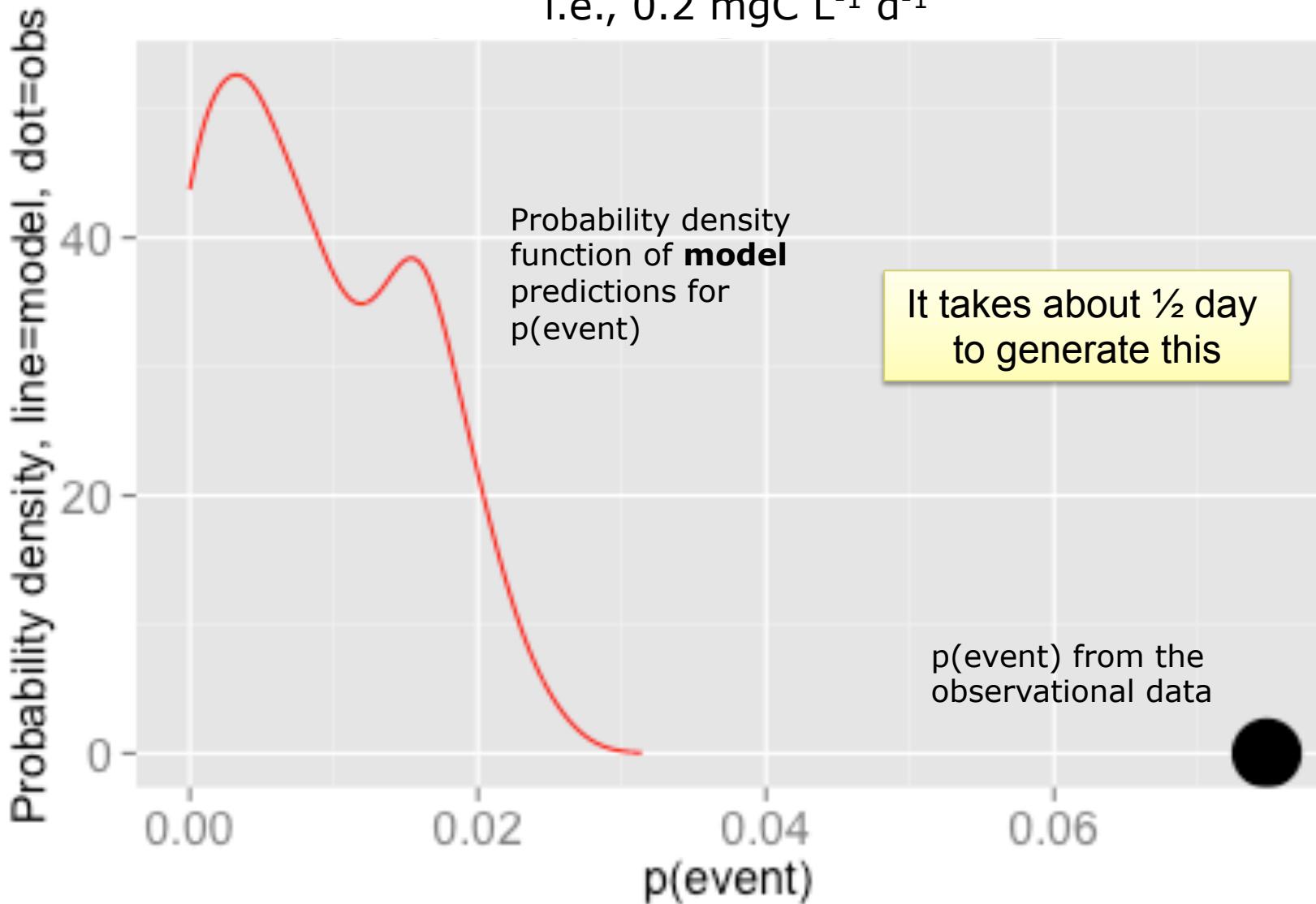
A) Phytoplankton time series



B) SAX representation of the probability distributions



# What is the probability of a bloom i.e., $0.2 \text{ mgC L}^{-1} \text{ d}^{-1}$



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## **Goals for supplemental proposal:**

1. Make available and usable new services, software and approaches to freshwater scientists
2. Expand the overlay technology beyond the existing PRAGMA-GLEON expedition
3. Grow the next generation of users by training students how to use GLM-AED to study lake water quality with hands-on modules
4. Assess the efficacy of integrated technology-science-education development in the classroom and in GLEON working groups

# New PRAGMA Partners

- Yoshio Tanaka (Information Technology Research Institute, AIST), co-lead of PRAGMA Resources Working Group
- Shinji Shimojo (Osaka University)
- Weicheng Huang (National Center for High-performance Computing), who has interest in the coordination of PRAGMA testbeds and proposed simulations and applications
- Kohei Ichikawa (NAIST), with interest in interconnecting IPOP network with OpenFlow network to expand the available resources

# Technology

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- Distributed resources are available
  - Desktops, servers, cloud; how to aggregate in user-friendly manner, with low administrative overhead?
- Local, familiar computer environments
  - Windows/MacOS, GLM, R
  - Present user's preferred environment for ease of use
- Technical approach
  - IPOP: overlay automatically creates virtual network; only requirement is to run software on endpoints
  - HTCondor: high-throughput computing job manager
  - GRAPLER: Web interface conveniently accessible from a user's desktop – R

# IP-over-P2P (IPOP) Overlay

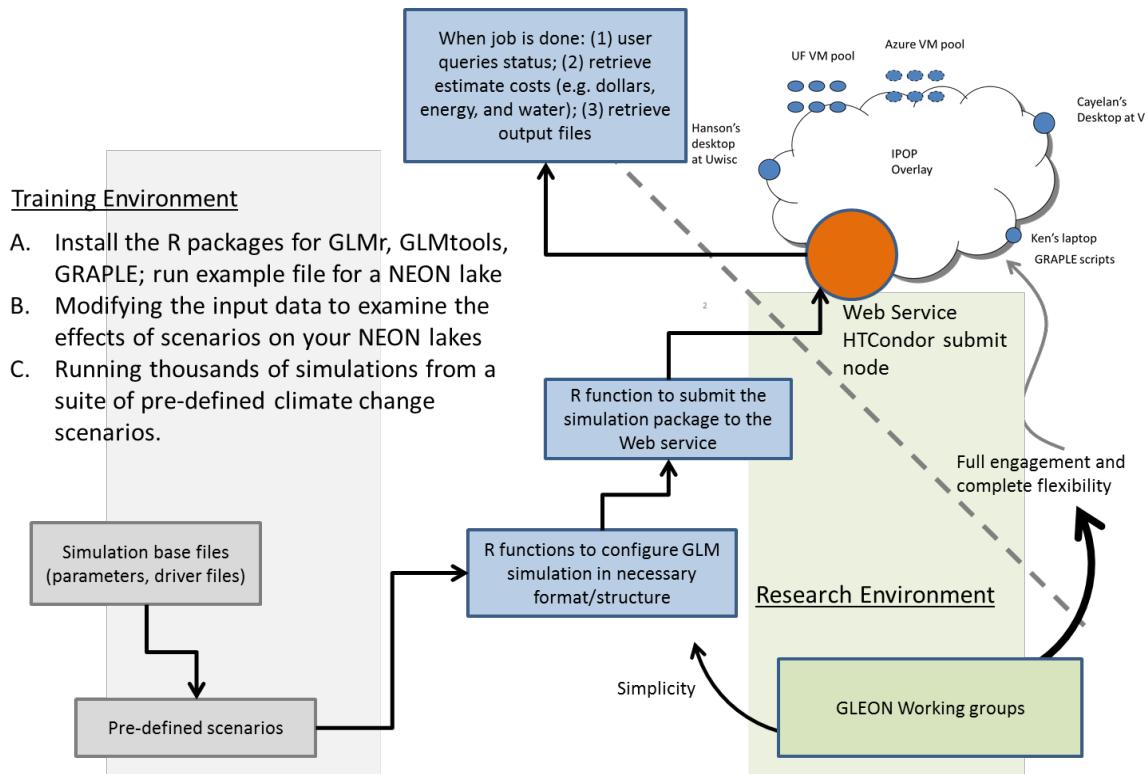
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- “User-Defined Networking”
  - SDN that users can deploy
    - User-level; easy to use
  - Software only needed at endpoints
    - Cloud VMs, personal computers, mobile devices
  - Map social network to virtual network links
    - E.g. GRAPLE researchers, students
  - Peer-to-peer VPN links
    - No centralized gateway
- Learn more about the open-source software:
  - <http://ipop-project.org>
  - Demo

# Technology Updates

## □ GRAPLER Web Service

- Expose simple R desktop interface to users
- Handle packaging of multiple simulations into Condor job, compression, and job submission



# Demonstration

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# Expanding GRAPLE globally

- We have developed GRAPLEr scripts as part of a teaching module to run the lake model in undergraduate and graduate classrooms
- Students manipulate climate and land use scenarios and then run the lake model to study their effects *in silico*

```
1 #DOC Model
2
3 setwd("~/Users/cayelan/Dropbox/ComputerFiles/Virginia_Tech/Falling Creek/2014 Data/OrganicCModel")
4 data<-read.csv("InputData_FCR_7Apr15.csv", header=TRUE)
5
6 data$date<-as.POSIXct(strptime(data$date, "%Y-%m-%d", tz="EST"))
7 #REMEMBER- think about adding in dt
8
9 simDays<-29 #need to interpolate the entire data frame so that we have daily obs for each variable
10
11 #parameters
12 lakeArea = 67000 #m^2
13 lakePer = 9500 #m
14 lakeDepth = 5 # mean depth
15 lakeVol = lakeArea * lakeDepth #m^3
16 #resTime = 1 #years
17 evap = 0.75 #m/year
18 HenryCO2 = 0.01
19 HenryCO2c = 0.04 #PAUL LOOK THIS UP
20
21 DOCE = data$DOC_0m_mgL[1] * data$Epilimnion_Vol_Adj_L[1] #mg/L concentration in lake
22 DOCH = data$DOC_9m_mgL[1] * data$Hypolimnion_Vol_Adj_L[1] #mg/L concentration in lake
23 CO2E = data$Epilimnetic_CO2_wutm[1] * HenryCO2 * 12/1000 * data$Epilimnion_Vol_Adj_L[1]
24 CO2H = data$Hypolimnetic_CO2_wutm[1] * HenryCO2*12/1000 * data$Hypolimnion_Vol_Adj_L[1]
25 O2E = data$Oxygen_Eepi_wutm[1] * data$Epilimnion_Vol_Adj_L[1]
26 O2H = data$Oxygen_Hypo_wutm[1] * data$Hypolimnion_Vol_Adj_L[1]
27 DOCq = data$DOC_Inflow_Conc_mgL[1] #mg/L concentration in inflowQ
28 #DOCdep = 300 #m/year shoreline/year shoreline deposition
29 DOCresp = 0.001 #/days respiration rate
30 DOChresp = 0.001 #/days respiration rate
31
32 #DOCsedt = OCresp*3 #/days sedimentation rate
33
34
35 #m3/day
36 #Qout = Qin - (LakeArea*evap/365) #m3/day
37
38 #lakes
39 results = data.frame(simDay = seq(1,simDays), DOCE = NA, DOCH = NA, CO2E = NA, CO2H=NA, O2E=NA, O2H=NA)#lakeOC = NA, load = NA, resp=NA)
40 results[1,2] = DOCE #mg/L
41 results[1,3] = DOCH
42 results[1,4] = CO2E
```



# Next steps

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- The first cohort of students at GLEON will be formally assessed to track their responses to using GLM and Web service + overlay technology
  - Monday workshop: Cayelan + Paul + Renato
- This module will be disseminated to 8 universities across the U.S. for testing in the fall and will be released publicly in 2016
- We have partnered with pedagogical experts to study how non-CS students use this technology  
→ will enable broad dissemination

# Acknowledgments

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- GRAPLE students
  - Craig Snortheim, Jon Doubek, Alex Gerling, Kate Hamre, Ryan McClure
- IPOP developers
  - Ken Subratie, Kyuho Jeong, Saumitra Aditya
- This material is based upon work supported in part by the National Science Foundation under Grants No. 1234983 and 1339737

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Factors Affecting Simulation Performance					
nSims	Duration	Resolution	Output	Runtime	Total Run Time
1000	9 mo	Daily	0.01 GB	140 min	140 min
1001	9 mo	8 hour	0.12 GB	200 min	200 min
1000	9 mo	1 hour	1.00 GB	700 min	700 min

Number of simulations in an experiment

Duration of the simulation

How frequently predictions are recorded

Output file size

Total run time

Too much for me and my laptop