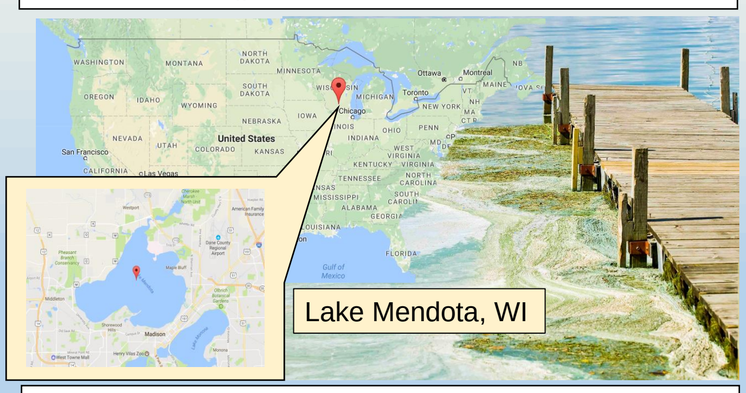
Numerical simulation modeling coupled to the GRAPLEr distributed computing platform provides insight into lake water quality responses to climate and land use change

Arianna I. Krinos[1], Renato J. Figueiredo[2], Paul C. Hanson[3], Amy L. Hetherington[1], Kensworth Subratie[2], Jaikrishna T. Sukumar[2], Cayelan C. Carey[1]

[1]Department of Biological Sciences, Virginia Tech, [2]Advanced Computing and Information Systems Laboratory, University of Florida, [3]Center for Limnology, University of Wisconsin-Madison

Key Points

- The GRAPLEr distributed computing platform makes it possible to analyze thousands of climate and land use scenarios to study nonlinear responses of water quality to anthropogenic change.
- We used GRAPLEr to run 100,000 simulations to study the effects of future climate and land use on Lake Mendota, Wisconsin, USA, a GLEON site.
- Increasing temperatures will favor the dominance of non-nitrogen-fixing cyanobacteria, which may increase toxin production and scums in Lake Mendota.
- Using distributed computing allows researchers to focus on analysis and expansion, thereby saving countless hours of valuable time and enhancing workflow for lake modeling.



Motivation

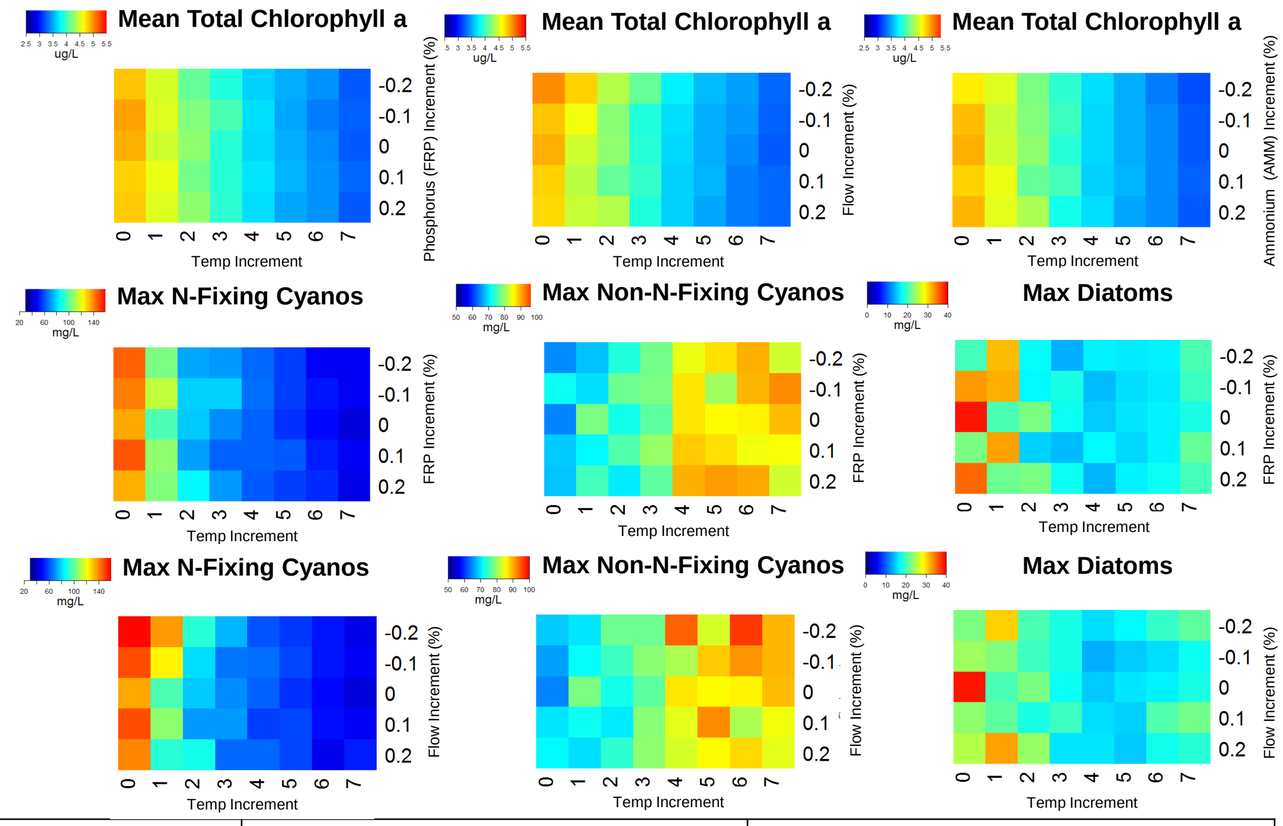
- Lakes provide many critical ecosystem services to humans, including drinking water, irrigation, hydropower, and recreation.
- Lakes are threatened by both changing climate and watershed land use, which may interact to decrease water quality.
- For example, human activities such as agriculture and land development have increased nitrogen and phosphorus loads in many lakes. Elevated nutrients can cause phytoplankton blooms, which result in surface scums, noxious odors, and promote the release of toxins dangerous to humans and pets.
- Simultaneously, much of North America is predicted to experience increased temperatures in the future, and climate modeling can yield estimates of this change.
- We need to analyze the effects of both changing climate and land use in concert to protect essential freshwater ecosystems and the benefits they provide.

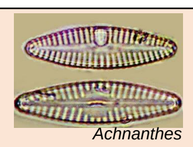
Results: Non-N-fixing cyanobacteria increase

Temperature surpasses nutrients as a driver of changes in lake productivity.

Non-nitrogen-fixing cyanobacteria will increase due to rising temperature; diatoms and nitrogen (N) fixers will decrease.

Changes to lake water volume have a disproportionate impact on the amplification or reduction of the trend.



Group	N-Fixing Cyanobacteria	Non-N-Fixing Cyanobacteria	Diatoms
Morphology	 *Aphanizomenon*  *Anabaena*	 *Microcystis (aeruginosa)*	  *Achnanthes*
Key Traits	Produce nitrogen that organisms can use (ammonium) from atmospheric N.	Generally unicellular with high growth rates; main toxin producers in Mendota	Play a key role at the base of the food web for higher trophic levels; colder optima temp.
Impact	Steady drop with increase in temperature.	Rise with increasing temperature, especially after several deg. warming.	Concentrations drop rapidly with increasing temperature.

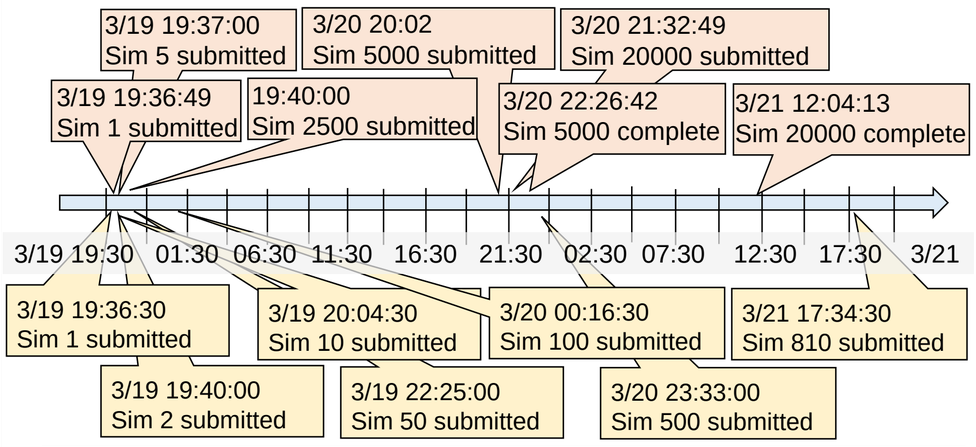
Credit: UNH PhycoKey

GRAPLEr is much faster than superhumans

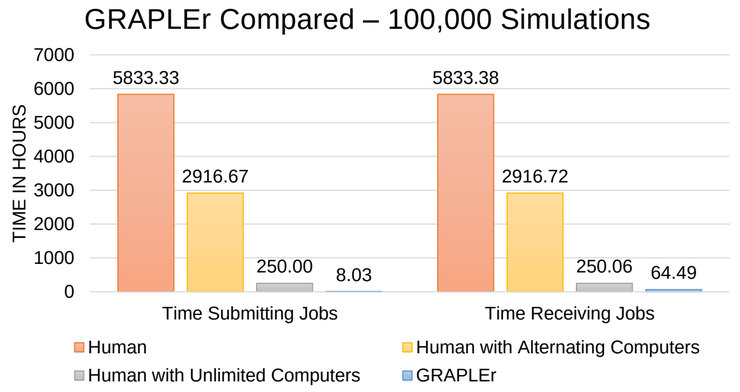
Why do lake modelers need distributed computing?

GRAPLEr distributed computing platform
- Scenarios are set up via JSON file
- Results automatically collated
- Can continue to submit simulations past 5000

For the first 20k simulations…



Personal Computer, individual GLM runs
- Must assume scenarios have been set up manually
- ~9 seconds to enter commands to start model; avg. 3:16 mins/run
- Estimated 3.5 minutes per run at superhuman capacity
- Normally only one GLM run possible at a time (start time of sim = end time of previous sim)



- GRAPLEr times include an allocation problem partway through the simulation
- The first 20,000 simulations were submitted and ran properly
- Simulations are submitted with increasing efficiency, but the more that are run, the longer the return time
- In practice, a constrained superhuman could expect to submit <100 simulations in an 8-hr day

The power of GRAPLEr for lake modeling

- The GRAPLEr platform has transformed our ability to conduct multi-factorial climate and land use scenario modeling. This GRAPLEr experiment made it possible to analyze an unprecedented 100,000 scenarios in 2 days. In comparison, running just 5,000 simulations manually would have taken 12 continuous days of superhuman capacity.
- Increases in nitrogen loads with increasing temperatures fuel a shift in dominance from nitrogen-fixing to non-nitrogen-fixing cyanobacteria. Diatoms are adversely impacted by changing temperatures and changes in lake water volume.
- The advent of GRAPLEr in the PRAGMA lake expedition has vastly increased lake researchers' computing capacity, allowing ecologists to devote energy and expertise to understanding complex interactions, rather than tedious setup and execution of established models.

Acknowledgements!

Generous support: NSF CNH 1517823, NSF PRAGMA 1234983

Feedback, help with writing, encouragement: Nicole Ward, Kait Farrell, Mary Lofton, Jon Doubek, and Ryan McClure