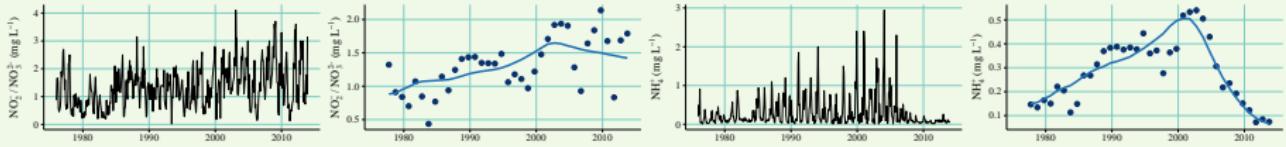


# Nutrients, estuaries, and coffee: Memoirs of a GED post-doc

Marcus W. Beck, Ph.D.

USEPA National Health and Environmental Effects Research Laboratory, Gulf Ecology Division, beck.marcus@epa.gov, Phone: 8509342480

August 28, 2017



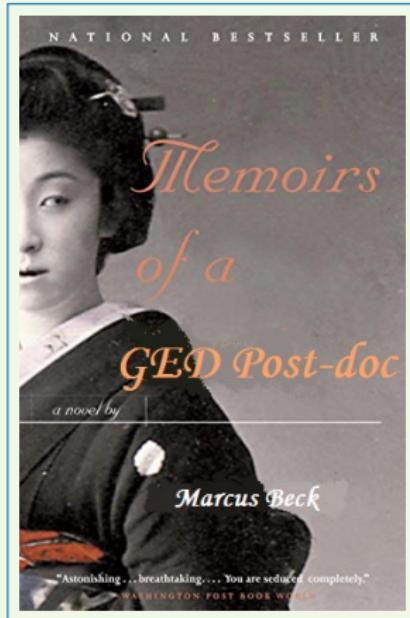
# Why are we here today?



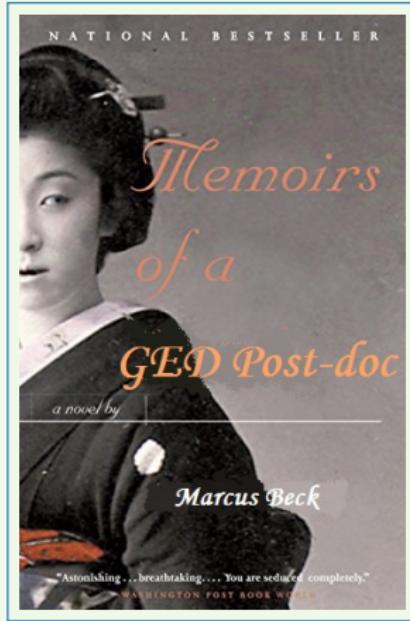
*Freedom is what you do with what's been done to you.*

– J. P. Sartre

# Why are we here today?

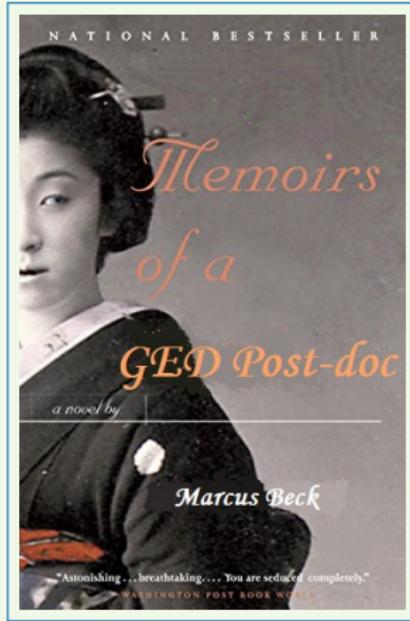


# Why are we here today?



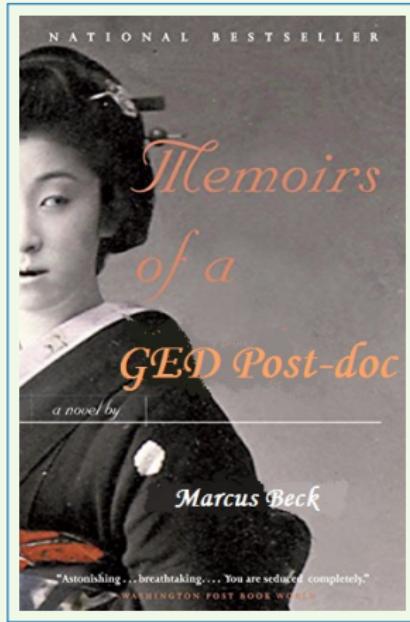
- Where did I come from?

# Why are we here today?



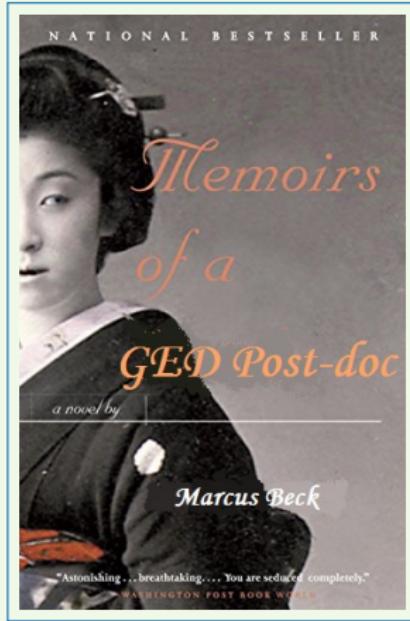
- Where did I come from?
- The ORISE experience

# Why are we here today?



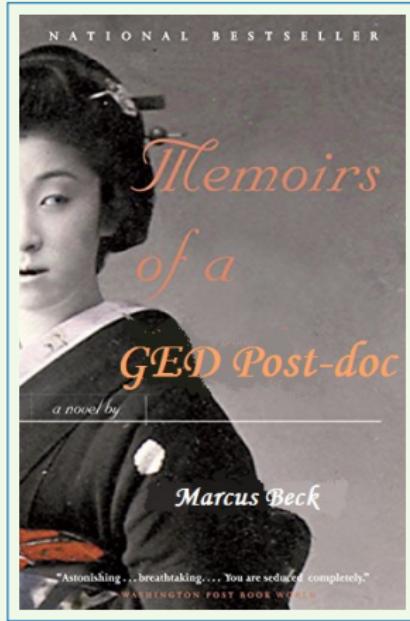
- Where did I come from?
- The ORISE experience
- The EPA experience

# Why are we here today?



- Where did I come from?
- The ORISE experience
- The EPA experience
- The next chapter

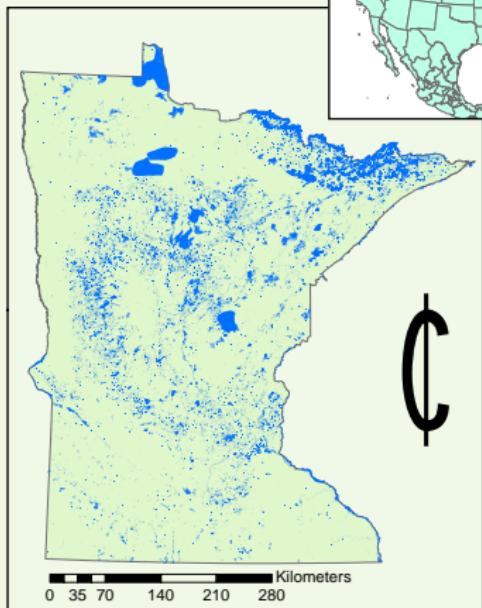
# Why are we here today?



- Where did I come from?
- The ORISE experience
- The EPA experience
- The next chapter
- Final thoughts/ramblings

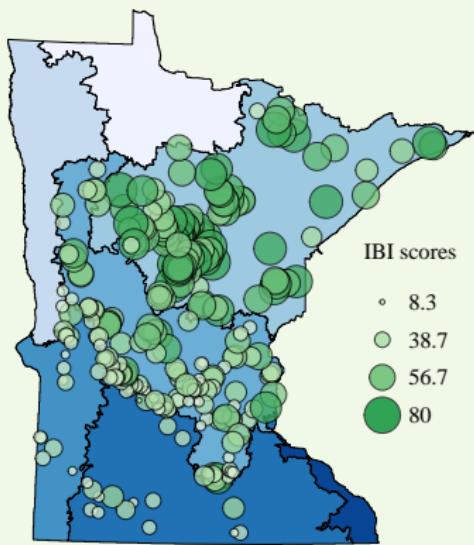
# Where did I come from?

Minnesota, the land of 11,842 lakes



# Where did I come from?

- Dataset of 332 vegetation surveys, courtesy of MNDNR  
[Beck et al., 2013, Beck et al., 2014]
- Environmental data describing lake characteristics and anthropogenic stressors



- lake surface area
- maximum lake depth
- trophic state index
- growing degree days
- percent agriculture in wshed
- percent impervious surfaces in wshed
- density of groundwater wells in wshed
- wshed area to lake area
- crop productivity index of wshed
- dock density
- ...

# The ORISE experience

*July 2013, moved to Pensacola*



# The ORISE experience



**OAK RIDGE INSTITUTE FOR  
SCIENCE AND EDUCATION**  
Managed by ORAU for DOE



# The ORISE experience



**OAK RIDGE INSTITUTE FOR  
SCIENCE AND EDUCATION**  
Managed by ORAU for DOE



OAK RIDGE ASSOCIATED UNIVERSITIES

- ORISE is a mysterious entity

# The ORISE experience



**OAK RIDGE INSTITUTE FOR  
SCIENCE AND EDUCATION**  
Managed by ORAU for DOE



- ORISE is a mysterious entity
- You are not an EPA employee

# The ORISE experience



**OAK RIDGE INSTITUTE FOR  
SCIENCE AND EDUCATION**  
Managed by ORAU for DOE



- ORISE is a mysterious entity
- You are not an EPA employee
- EPA employees cannot tell you what to do

# The ORISE experience



**OAK RIDGE INSTITUTE FOR  
SCIENCE AND EDUCATION**  
Managed by ORAU for DOE



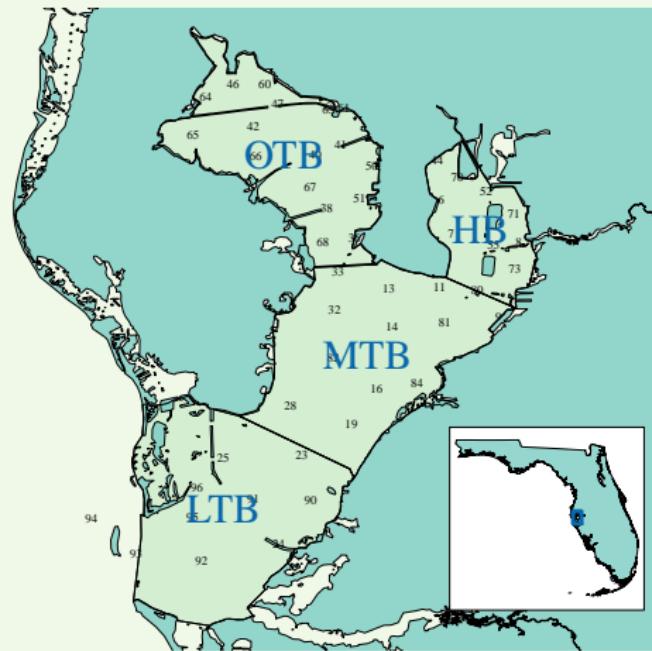
- ORISE is a mysterious entity
- You are not an EPA employee
- EPA employees cannot tell you what to do
- You are not responsible for anything

# The ORISE experience

## Tampa Bay trend analysis

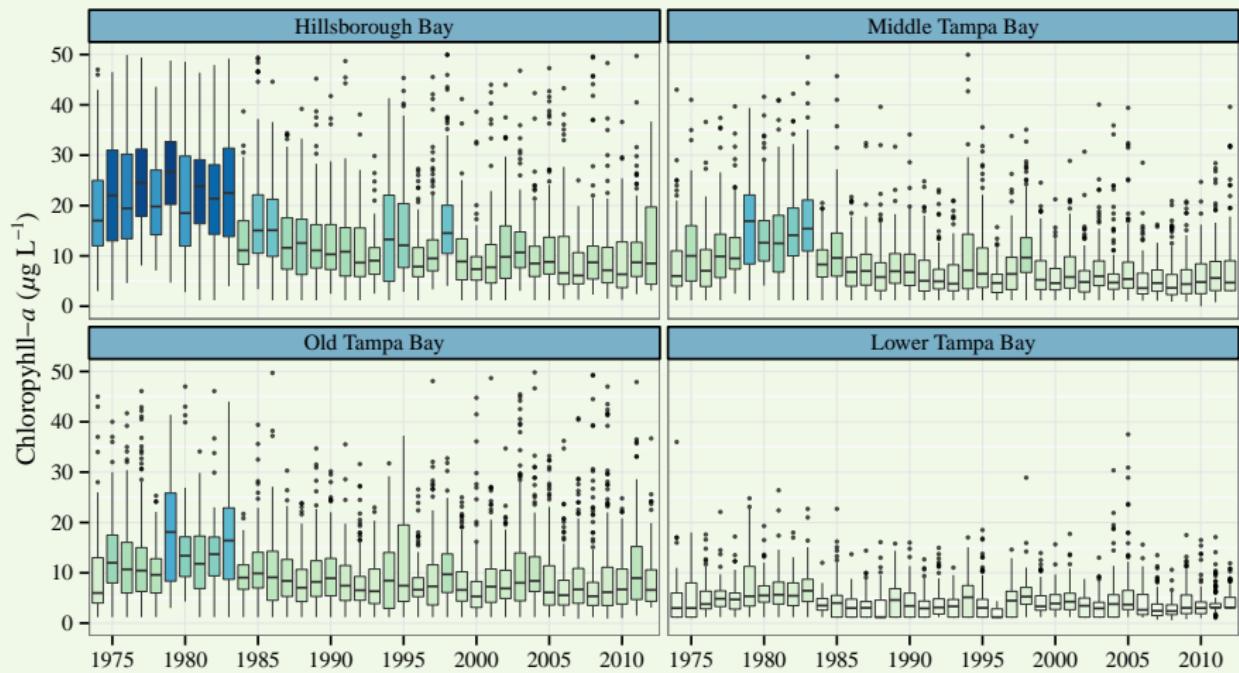
- Four bay segments
- Monthly wq data at 50 stations from 1974 to present
- Longitudinal profile of nutrient load and salinity

Data from [TBEP (Tampa Bay Estuary Program), 2011]



# The ORISE experience

## Tampa Bay trend analysis



# The ORISE experience

## Tampa Bay trend analysis

### Study objective

Adapt and apply a nutrient response model for estuaries that leverages the descriptive capabilities of large datasets [Beck and Hagy III, 2015]

# The ORISE experience

## Tampa Bay trend analysis

### Study objective

Adapt and apply a nutrient response model for estuaries that leverages the descriptive capabilities of large datasets [Beck and Hagy III, 2015]

### Questions of concern – Can we...

- ...provide a natural history of water quality that is temporally consistent with drivers of change?

# The ORISE experience

## Tampa Bay trend analysis

### Study objective

Adapt and apply a nutrient response model for estuaries that leverages the descriptive capabilities of large datasets [Beck and Hagy III, 2015]

### Questions of concern – Can we...

- ...provide a natural history of water quality that is temporally consistent with drivers of change?
- ...improve our understanding of the nutrient-response paradigm in estuaries?

# The ORISE experience

## Tampa Bay trend analysis

How does it work?

$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

*N*: nitrogen (or other response endpoint)

*t*: time

*Sal*: Salinity (or other flow-related variable)

# The ORISE experience

## Tampa Bay trend analysis

How does it work?

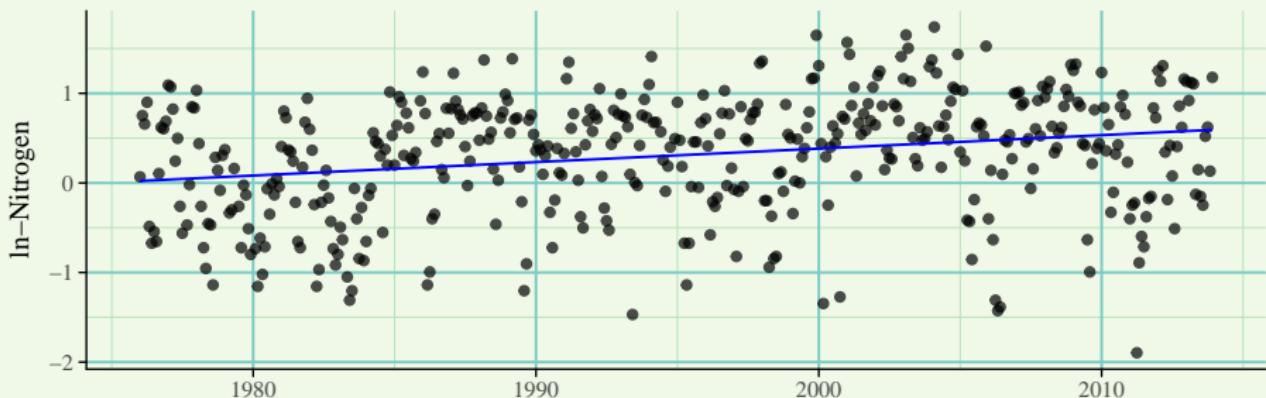
$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

$N$ : nitrogen (or other response endpoint)

$t$ : time

$Sal$ : Salinity (or other flow-related variable)

$\ln(N) \sim t$



# The ORISE experience

## Tampa Bay trend analysis

How does it work?

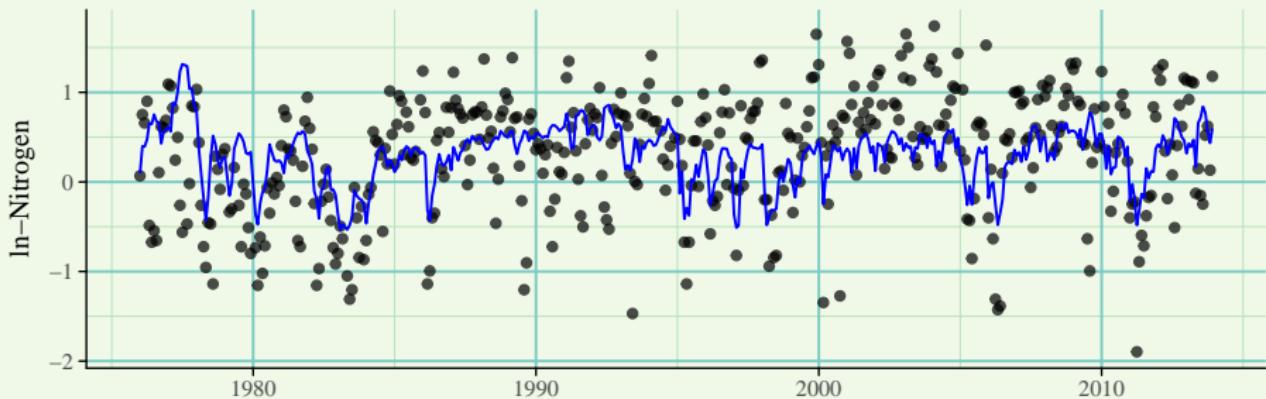
$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

$N$ : nitrogen (or other response endpoint)

$t$ : time

$Sal$ : Salinity (or other flow-related variable)

$\ln(N) \sim Sal$



# The ORISE experience

## Tampa Bay trend analysis

How does it work?

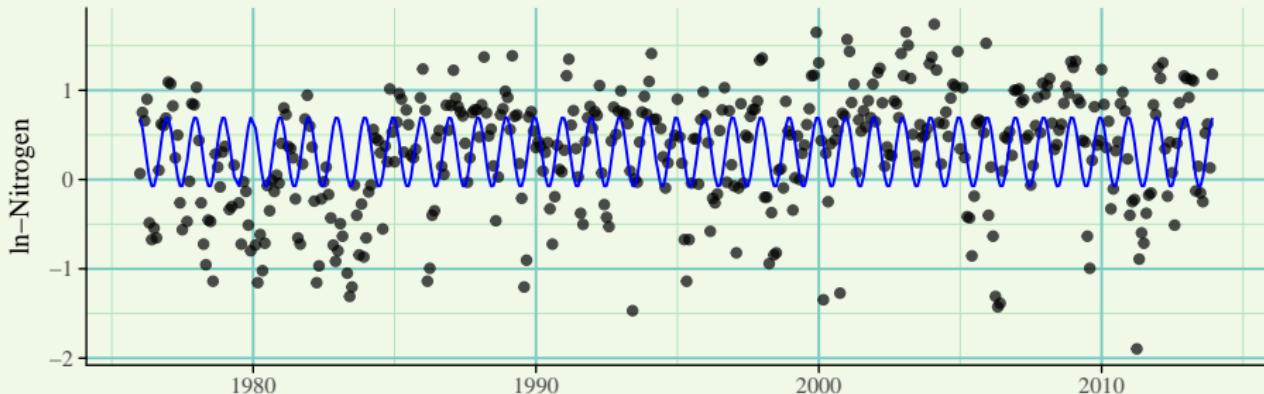
$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

$N$ : nitrogen (or other response endpoint)

$t$ : time

$Sal$ : Salinity (or other flow-related variable)

$$\ln(N) \sim \cos(2\pi * t) + \sin(2\pi * t)$$



# The ORISE experience

## Tampa Bay trend analysis

How does it work?

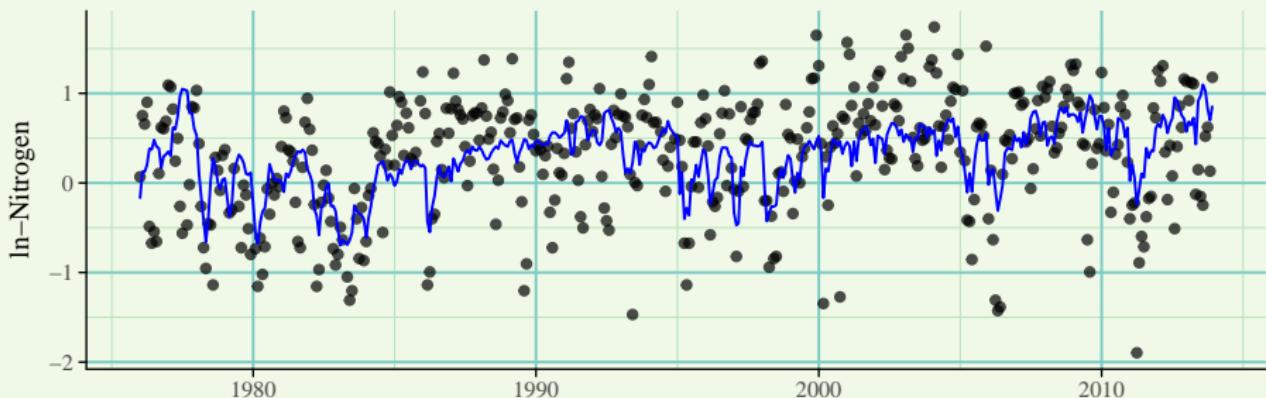
$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

$N$ : nitrogen (or other response endpoint)

$t$ : time

$Sal$ : Salinity (or other flow-related variable)

$$\ln(N) \sim t + Sal$$



# The ORISE experience

## Tampa Bay trend analysis

How does it work?

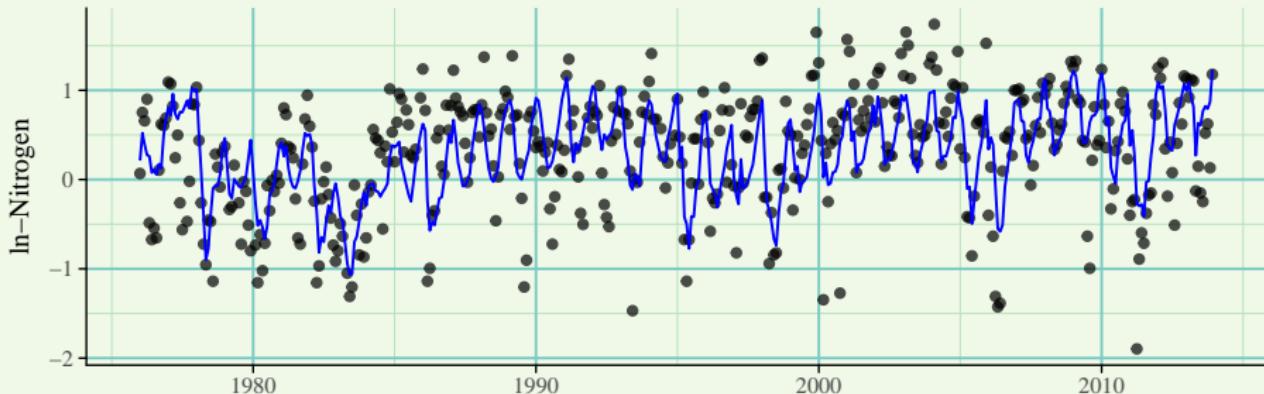
$$\ln(N) = \beta_0 + \beta_1 t + \beta_2 Sal + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$

$N$ : nitrogen (or other response endpoint)

$t$ : time

$Sal$ : Salinity (or other flow-related variable)

$$\ln(N) \sim t + Sal + \cos(2\pi * t) + \sin(2\pi * t)$$



# The ORISE experience

## Tampa Bay trend analysis

**Points:** observed time series (black are weighted, grey is zero weight)

**Green point:** observation at the center of the regression

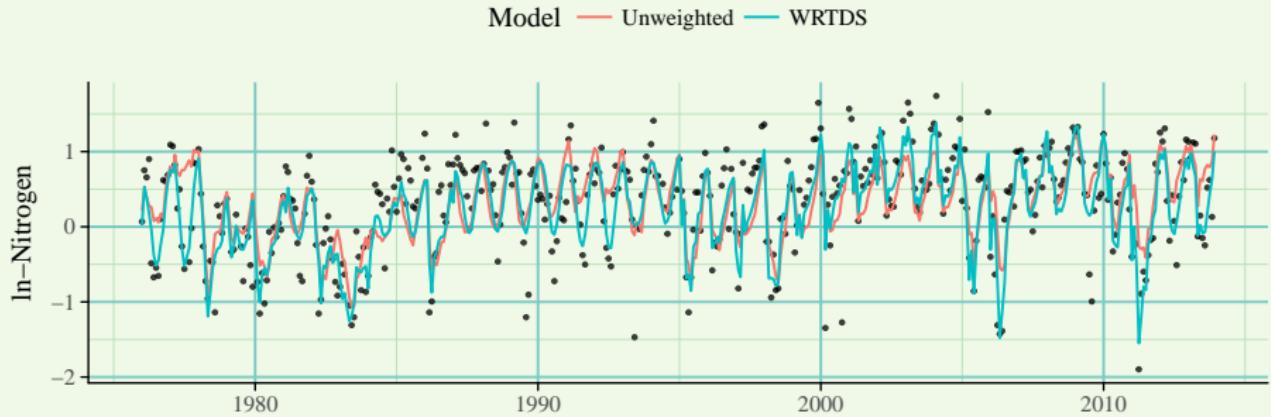
**Blue line:** Global model with weights specific to the window

**Red line:** Accumulated WRTDS model

# The ORISE experience

## Tampa Bay trend analysis

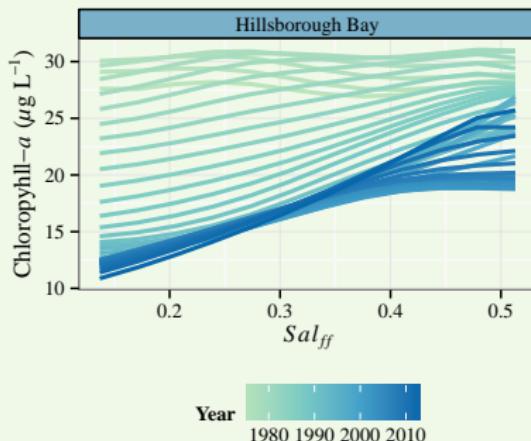
RMSE fit for unweighted = 0.58, WRTDS = 0.36



# The ORISE experience

## Tampa Bay trend analysis

Because the model is dynamic, we have parameters describing the relationship of chlorophyll with other factors specific to different time periods



- Early period (light blue) - point-sources
- Late period (dark blue) - non-point sources
- Chlorophyll shows increasing response to freshwater input in recent years

# The ORISE experience

## Tampa Bay trend analysis

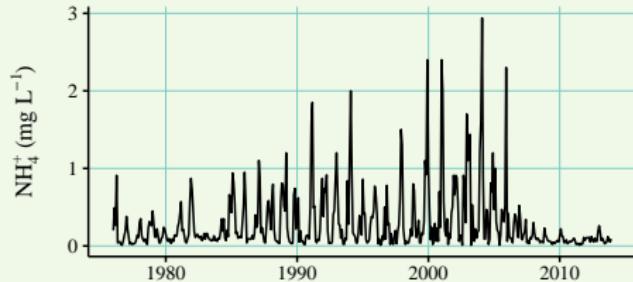
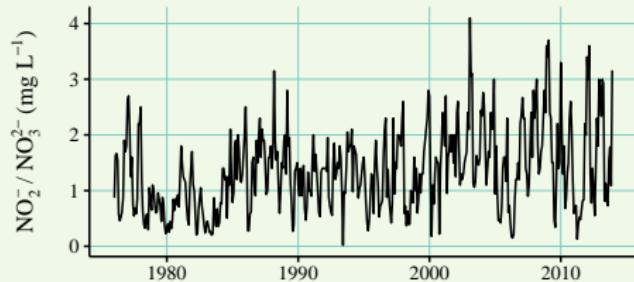


Figure : Observed nitrogen time series at P8 (SF Bay Delta RMP)

# The ORISE experience

## Tampa Bay trend analysis

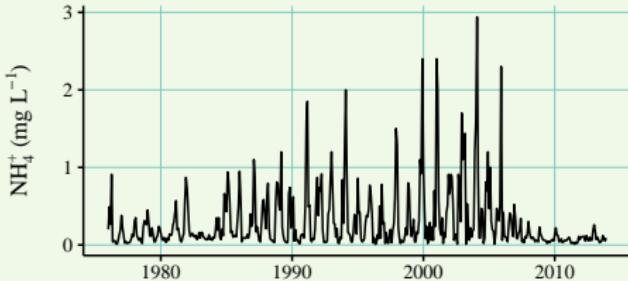
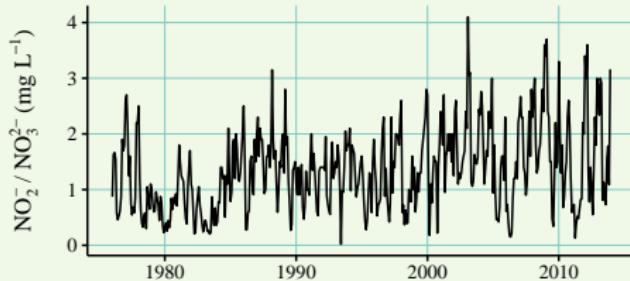


Figure : Observed nitrogen time series at P8 (SF Bay Delta RMP)

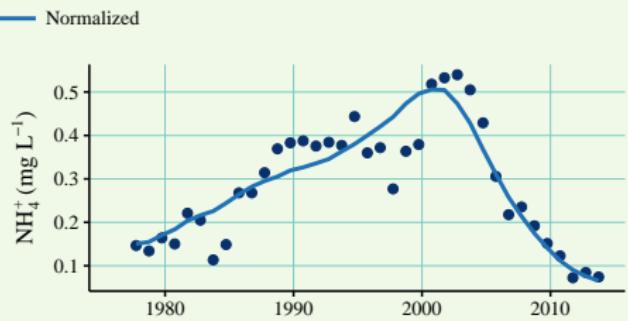
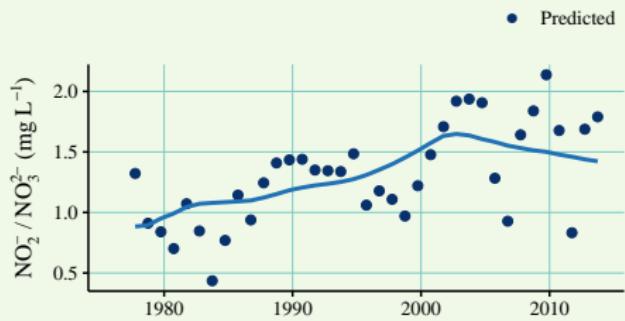


Figure : Annual predicted and flow-normalized nitrogen from WRTDS.

# The ORISE experience

## Time series detiding

The ‘Odum’ open-water method has been used for decades to estimate rates of ecosystem metabolism [Odum, 1956]

$$\frac{\delta DO}{\delta t} = P - R + D$$

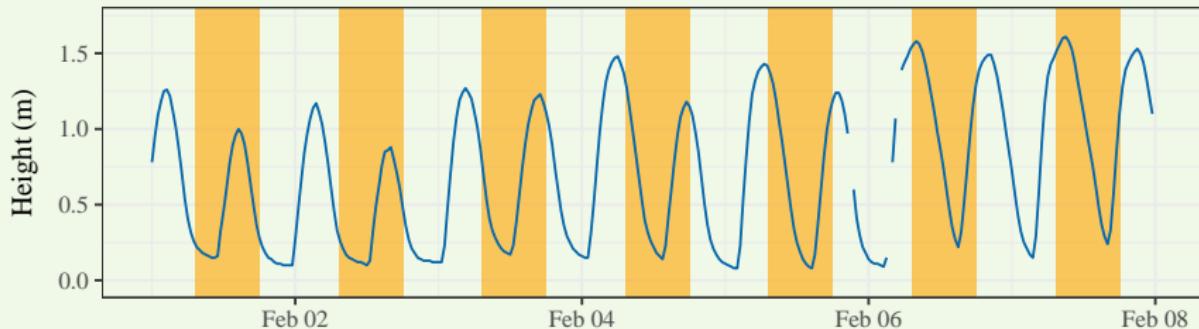
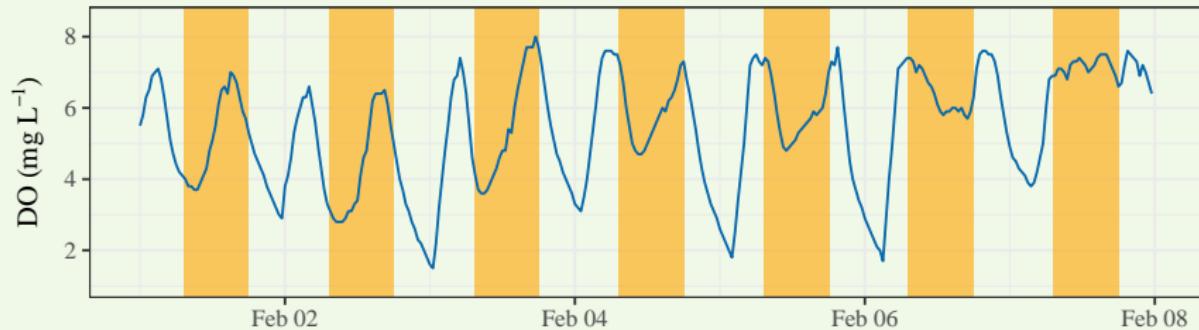
Metabolic rates provide a measure of productivity in a system - are estuaries sources or sinks of organic matter? [Caffrey et al., 2013]

Applications to estuarine monitoring data have been somewhat successful - why??

# The ORISE experience

## Time series detiding

The ‘Odum’ method assumes DO represents biological processes...



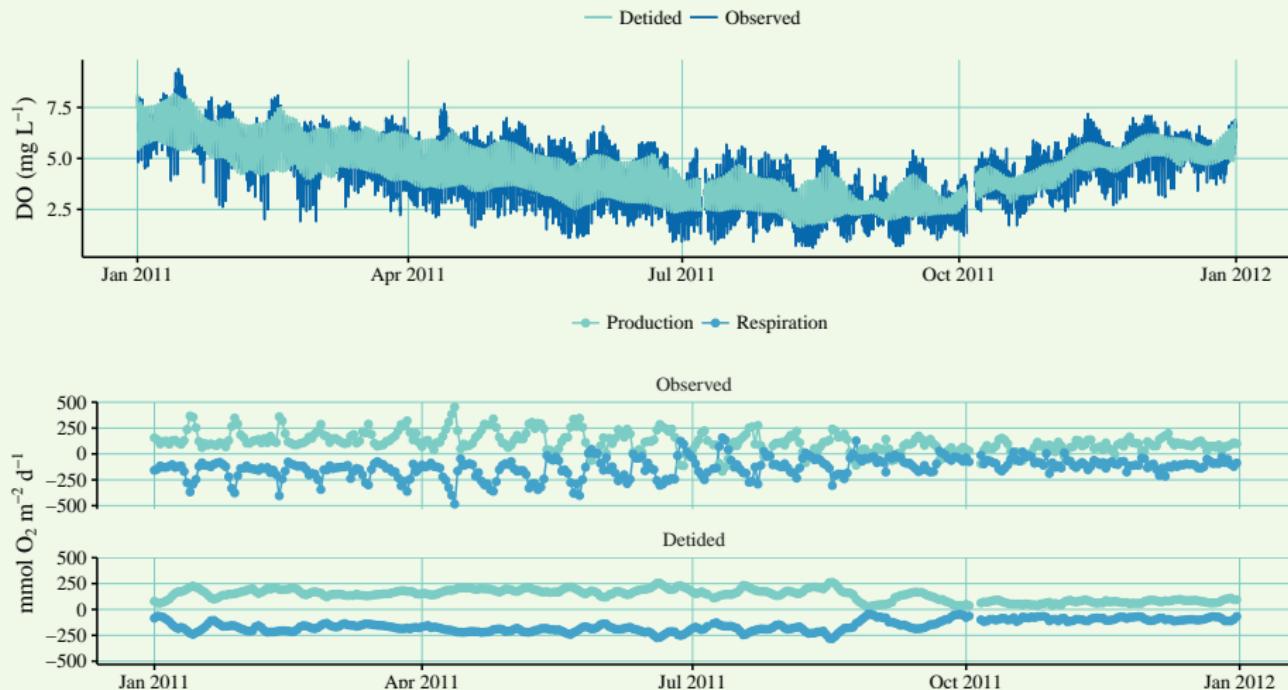
# The ORISE experience

## Time series detiding

# The ORISE experience

## Time series detiding

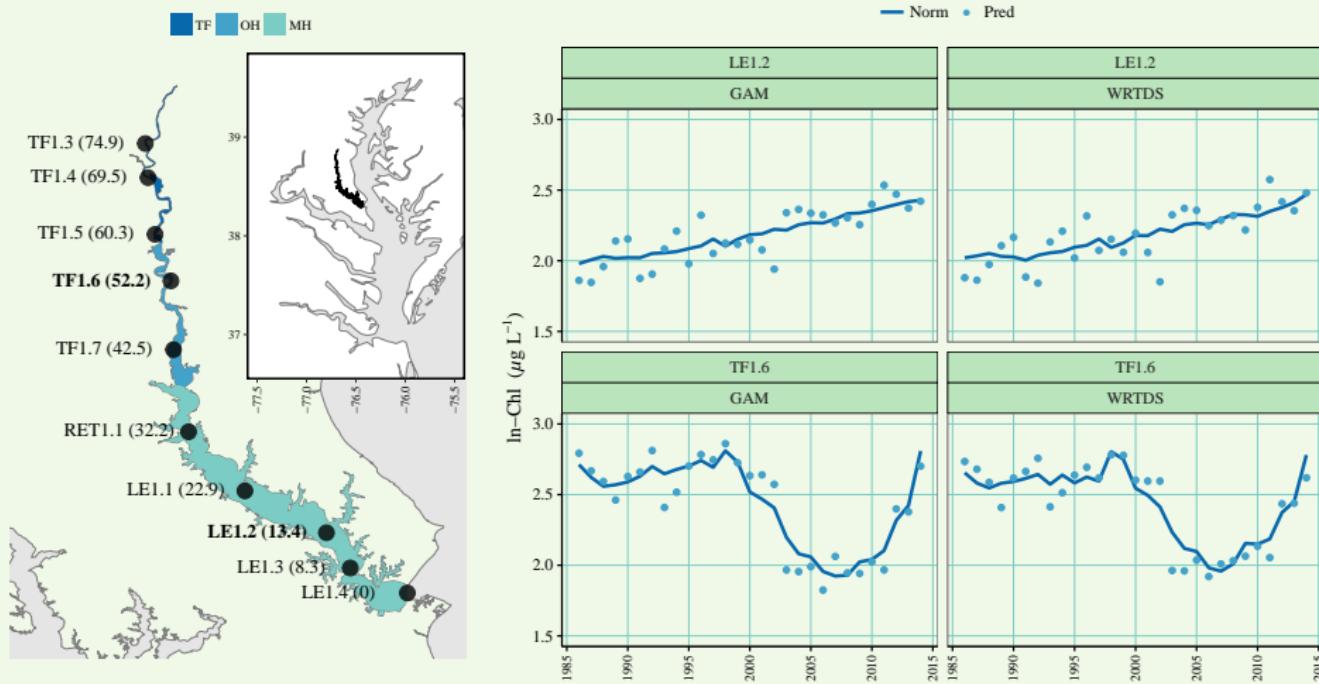
### DO time series and ecosystem metabolism [Beck et al., 2015]



# The ORISE experience

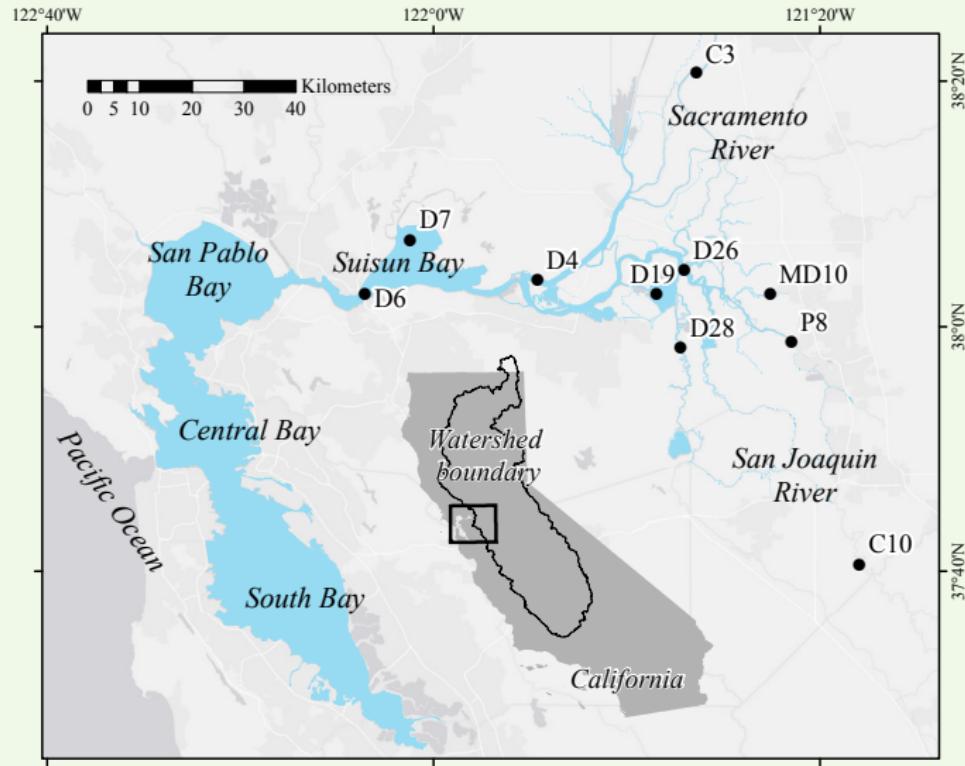
## Additional WRTDS applications

### Comparing WRTDS and GAMs for trend evaluation [Beck and Murphy, 2017]



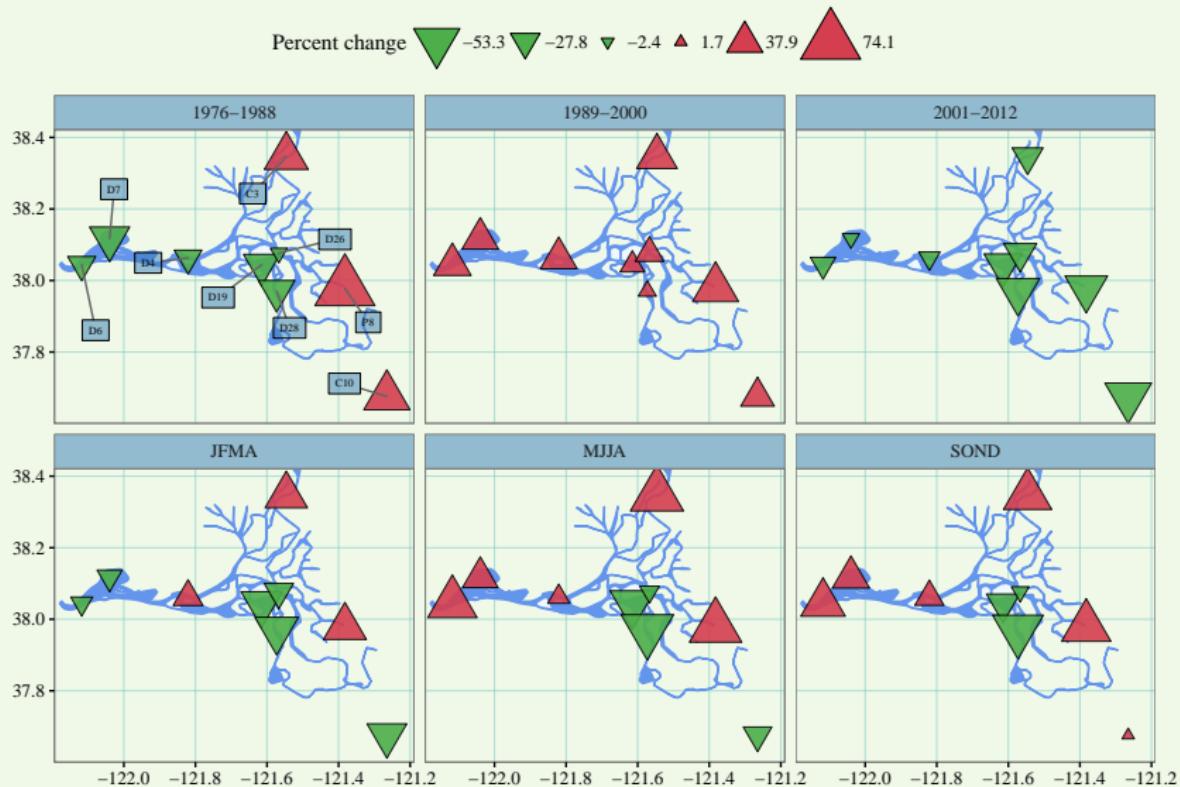
# The ORISE experience

## Additional WRTDS applications - DIN changes in Delta



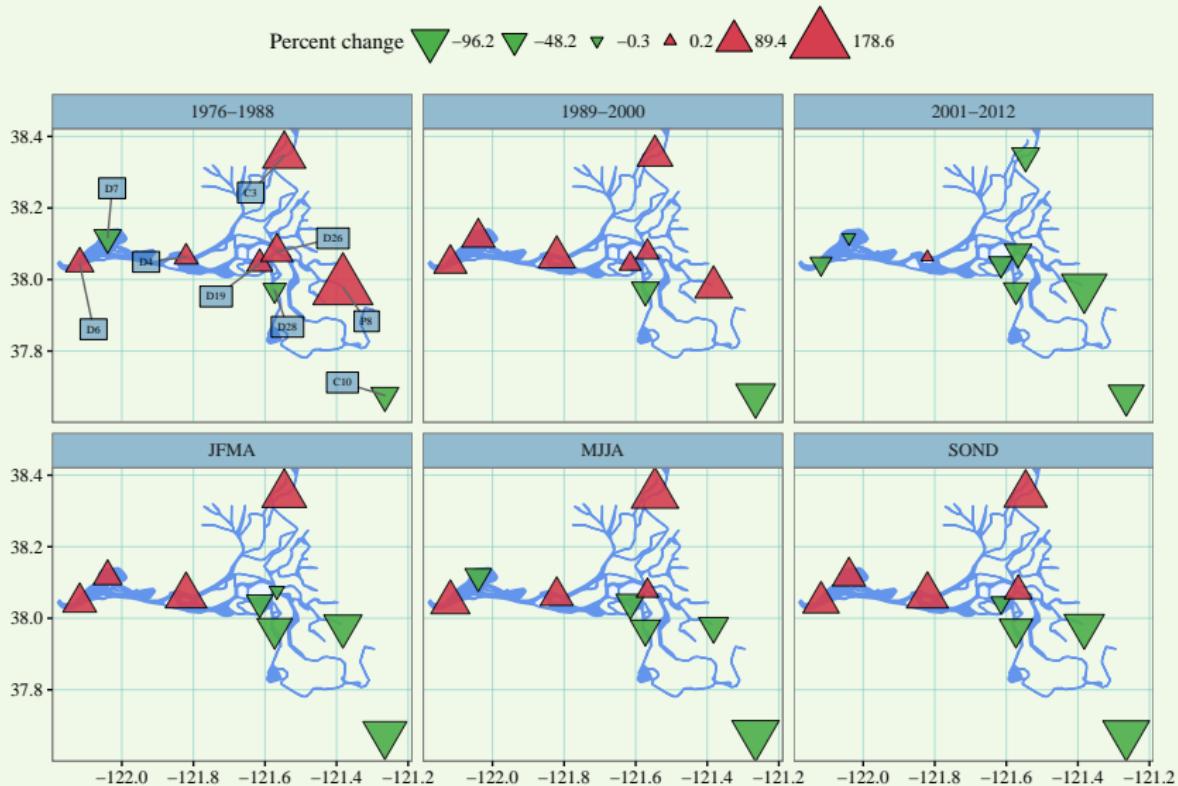
# The ORISE experience

## Additional WRTDS applications - ammonium changes in Delta



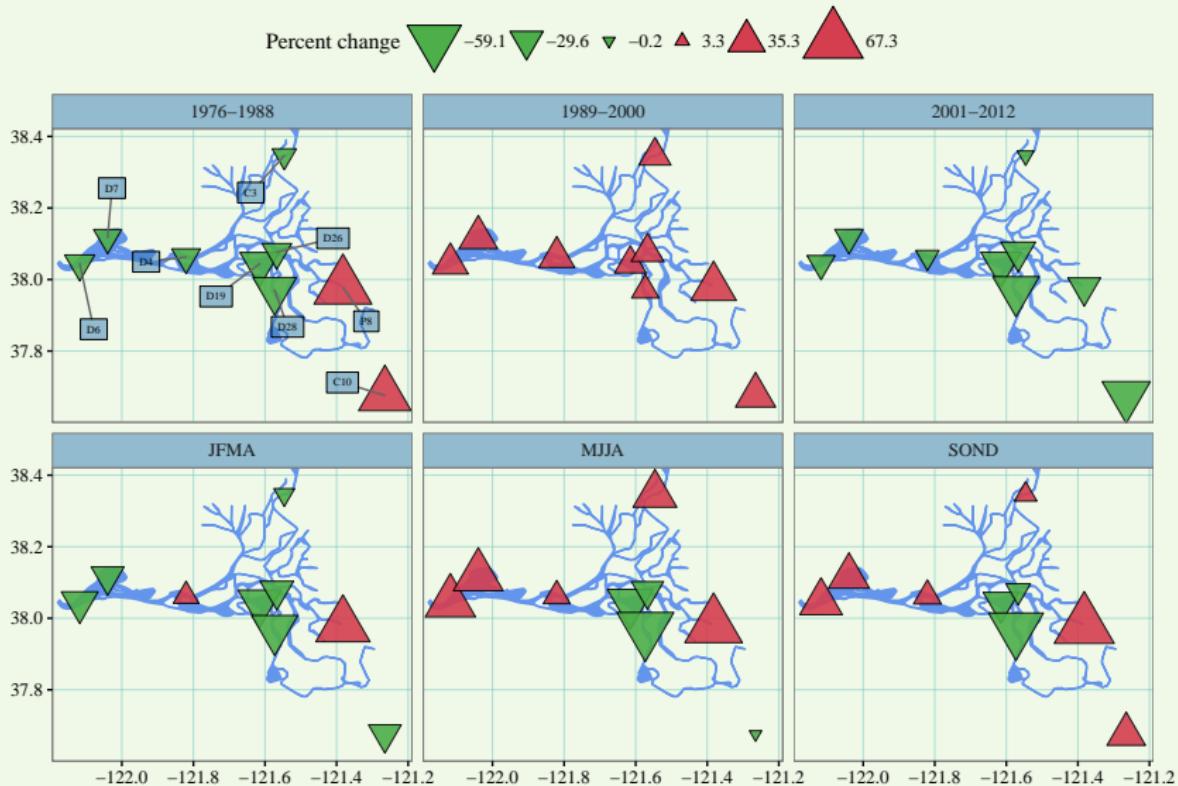
# The ORISE experience

## Additional WRTDS applications - nitrite/nitrate changes in Delta



# The ORISE experience

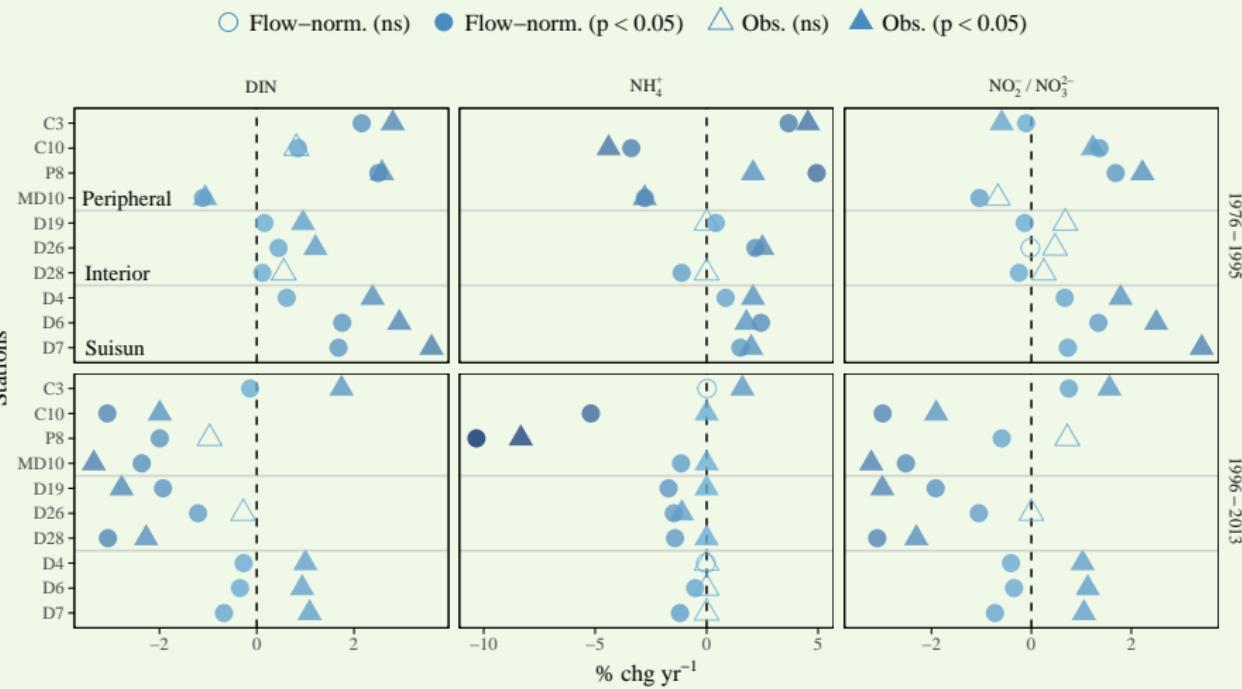
## Additional WRTDS applications



# The ORISE experience

## Additional WRTDS applications

Better description of nutrient endpoints can change conclusions



# The EPA experience



*R-term post-doc, Dec. 2015*

# The EPA experience



*R-term post-doc, Dec. 2015*

- You are a federal employee

# The EPA experience



*R-term post-doc, Dec. 2015*

- You are a federal employee
- You are not a permanent federal employee

# The EPA experience



*R-term post-doc, Dec. 2015*

- You are a federal employee
- You are not a permanent federal employee
- You can't tell contractors what to do

# The EPA experience



*R-term post-doc, Dec. 2015*

- You are a federal employee
- You are not a permanent federal employee
- You can't tell contractors what to do
- You move out of cubeland

# The EPA experience

## **3.01D** Watershed Sustainability

- Coral Biocriteria development

## **4.02A** Microbial Indicators

- Data munging

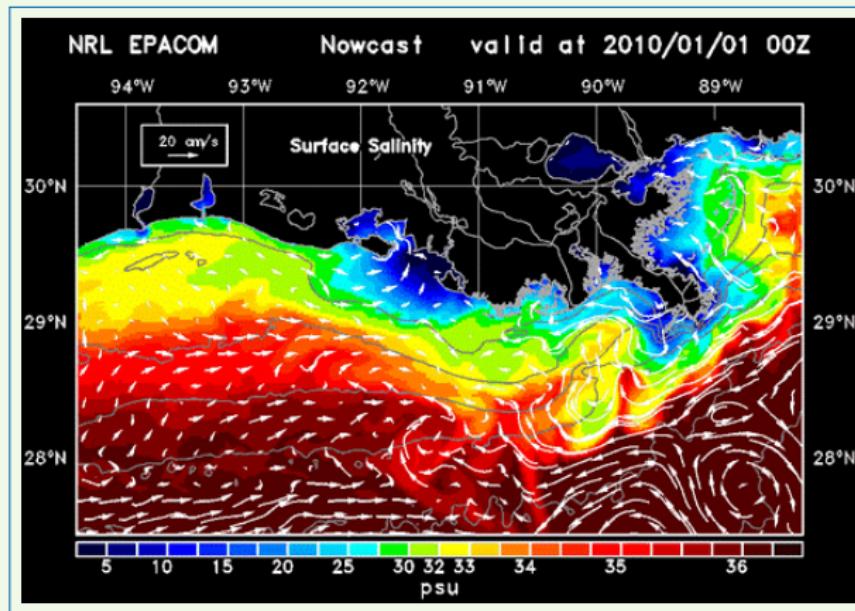
## **4.02B** Nutrient Response and Recovery

- Simulation modelling of NGOM hypoxia

# The EPA experience

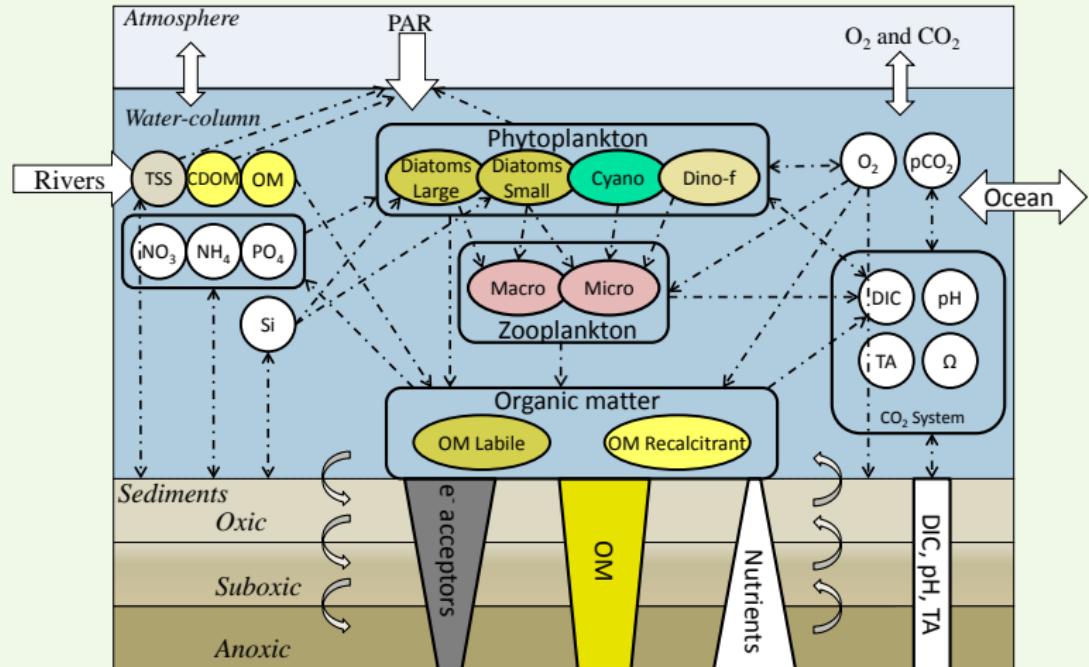
## 4.02B Nutrient Response and Recovery

### *Community General Ecology Model*



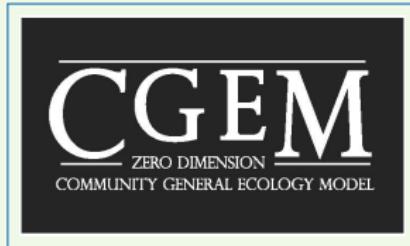
# The EPA experience

## 4.02B Nutrient Response and Recovery

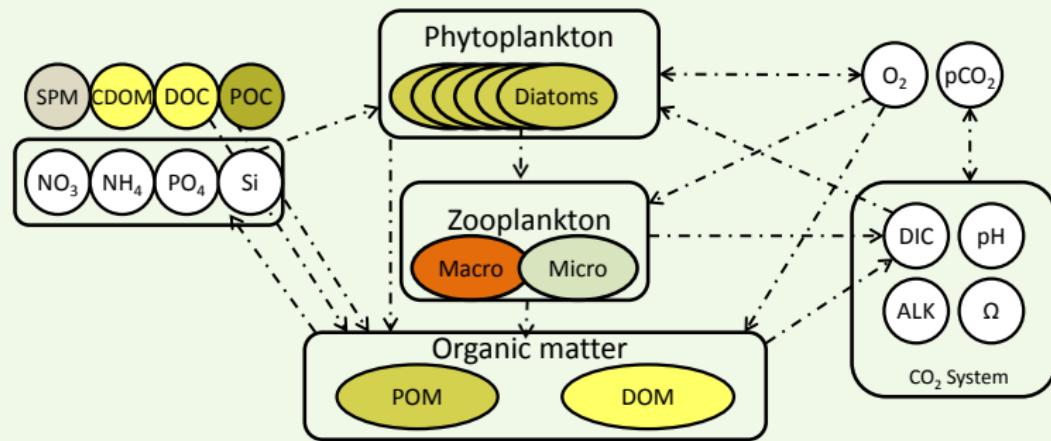


# The EPA experience

## 4.02B Nutrient Response and Recovery



- 36 state variables
- 108 structural equations
- 251 parameters



# The EPA experience

## 4.02B Nutrient Response and Recovery

### ***Basic concepts:***

Models seek to provide generality, precision, realism [Levins, 1966]

We can evaluate model uncertainty to address what a model should provide in this context

***Parameter uncertainty*** - uncertainty in the parameter space that provides bounds on structural equations

# The EPA experience

## 4.02B Nutrient Response and Recovery

### *Assumptions:*

- Parameter values based on field/lab data, literature, expert judgment
- Precision/accuracy limitations due to model domain, reproducibility
- Models are over-parameterized to address all objectives

# The EPA experience

## 4.02B Nutrient Response and Recovery

***Objective:*** Evaluate FishTank as 0D unit for larger CGEM model, provide guidance for further refining or application to new environments

- Local sensitivity analysis and identifiability
- Parameter selection heuristics

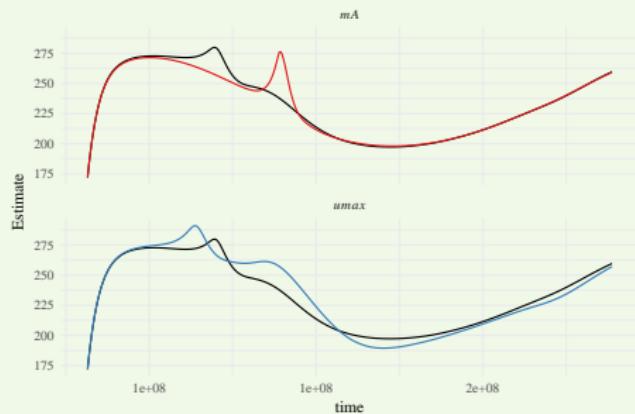
# The EPA experience

## 4.02B Nutrient Response and Recovery

**Method:** Local sensitivity analysis, single perturbation of model parameters [Soetaert and Petzoldt, 2010]

$$S_{ij} = \frac{\partial y_i}{\partial \Theta_j} \cdot \frac{w_{\Theta_j}}{w_{y_i}}$$

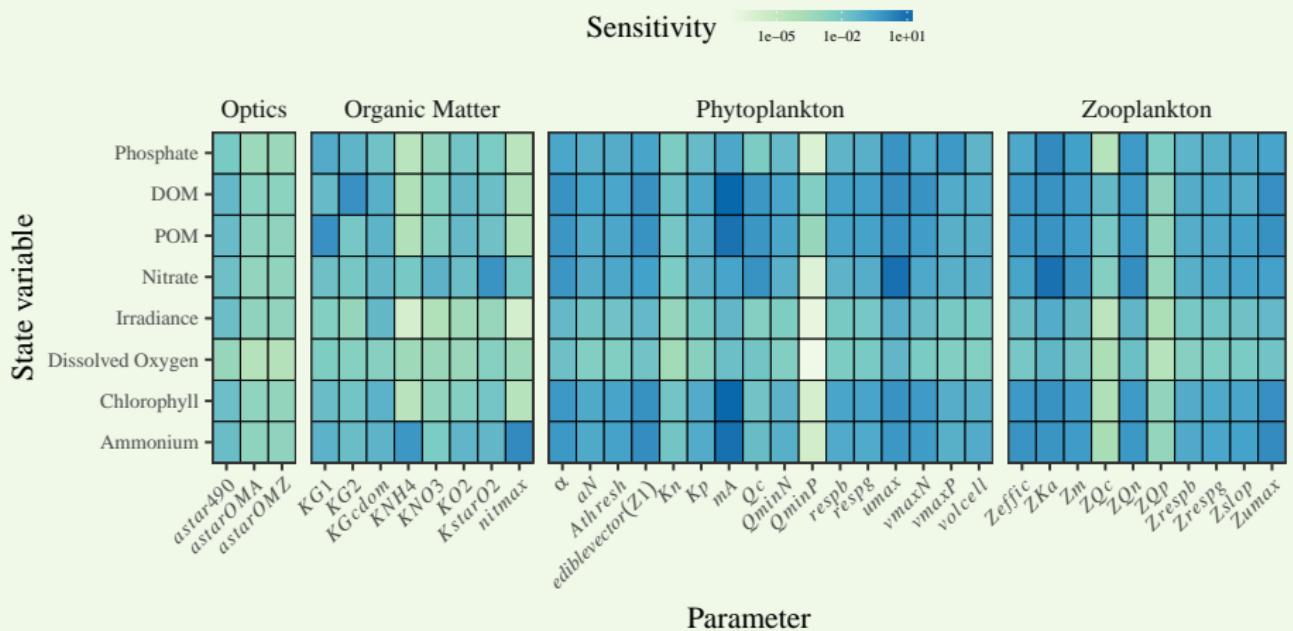
$$L_j = \sum |S_{ij}| / n$$



timestep	default	umax	mA
1	172.0	172.0	172.0
2	183.3	183.3	183.3
3	193.3	193.3	193.4
4	202.2	202.1	202.2
5	210.0	209.9	210.1
6	217.0	216.9	217.1

# The EPA experience

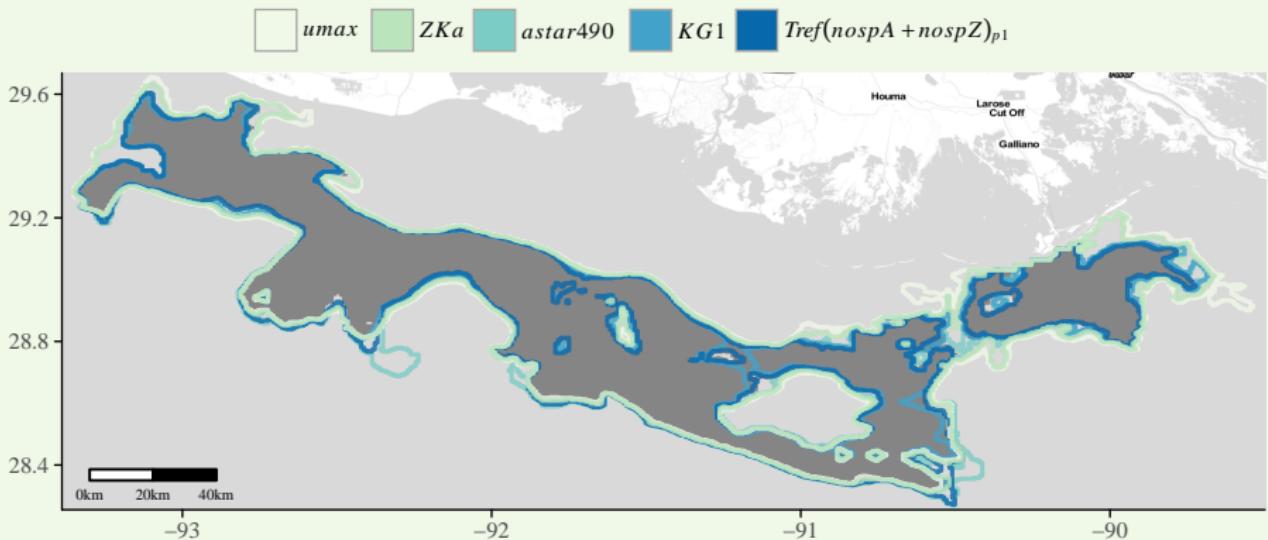
## 4.02B Nutrient Response and Recovery



# The EPA experience

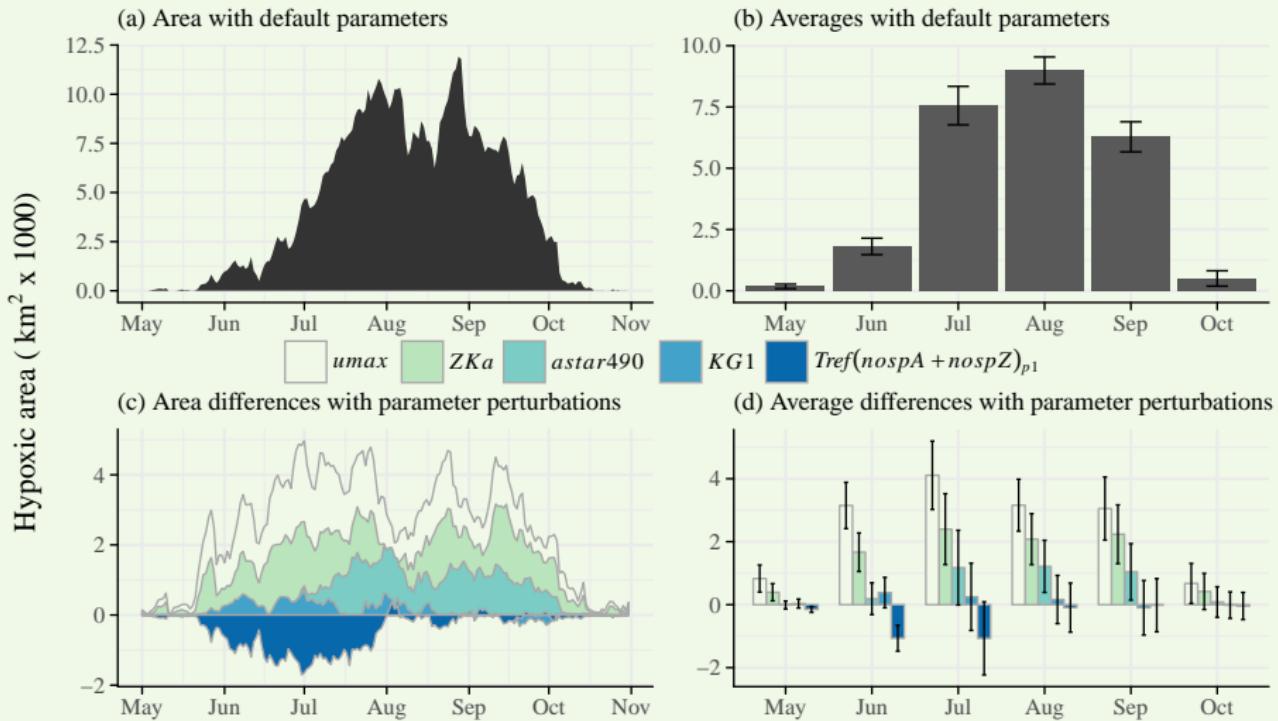
## 4.02B Nutrient Response and Recovery

*Estimated areal extents on August 28, default extent in grey*



# The EPA experience

## 4.02B Nutrient Response and Recovery



# The EPA experience

## 4.02B Nutrient Response and Recovery

### *Ongoing*

- How do these analyses depend on interactions between variables?
- How can this inform evaluation of structural or observational uncertainty?
- Can we use this information to develop better understanding of hypoxia development?
- Manuscript in revision, interactive GUI for FishTank

# The EPA experience

## 4.02B Nutrient Response and Recovery



This application runs the FishTank model as part of the Coastal Gulf Ecology Model (CGEM). CGEM calculates a set of bio-geo-chemical equations based on the Eldridge and Roelke model (Eldridge and Roelke, 2010). The equations have been enhanced by J. Lehrter (Lehrter, et al. 2014). A comprehensive light model has been added by B. Penta of the Naval Research Lab (NRL) (Penta et al., 2008). Hydrodynamics and transport were added by D.S. Ko of NRL (Ko et al., 2008). The model aims to explain the seasonal appearance of a large hypoxic zone off of the Louisiana continental shelf (LCS). Input parameters are selected on the left tab and the model is run by clicking the button to the left. Results are viewed as time series plots for 33 different state variables on the right tab.

Select parameters

Select initial conditions

Model output

### Simulation specifics

#### Series length

2006-01-01 to 2006-12-31

- dT (timestep, seconds); dT\_out (output interval, seconds)

300                    86400

- How cell Location is specified: 0==long-lat 1==grid-units

0

- Cell i,j coord (if grid-units) or longcent,latcent vals (if long-lat)

-92.39                    29.03

### Switches in GEM

Which Fluxes, toggle on(1) off(0): Atmospheric Deposition of Nutrients, Instant Remineralization in Bottom Layer, Sediment Diagenesis Model

0                    0                    0                    0                    0                    0

0                    0

Which\_temperature: 1==Sigmoidal, 2==Optimum Temp. Thresh., 3==Arrhenius

1

Which\_uptake: 1==Michaelis-Menten, 2==Geider (needs nfQs), 3==Roelke

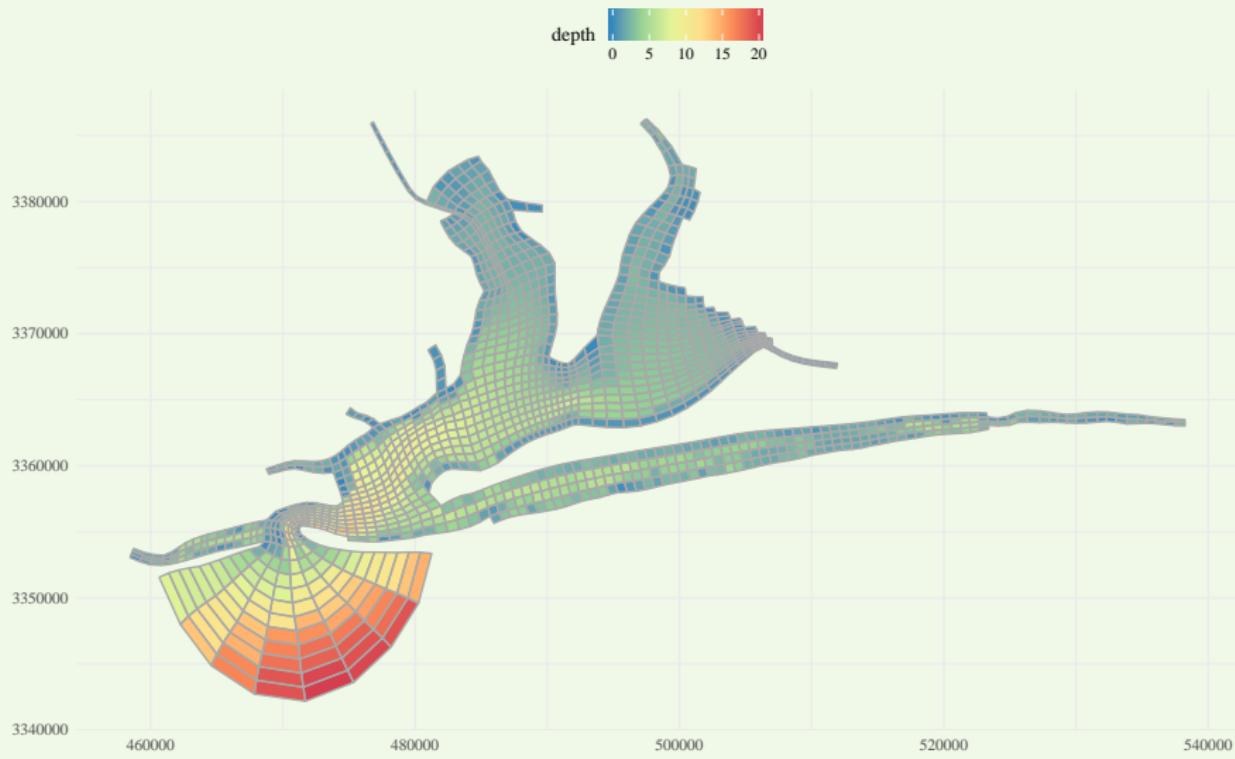
1

Which\_quota: 1==Droop, 2==Nyholm, 3==Flynn, Nutrient dependant growth

1

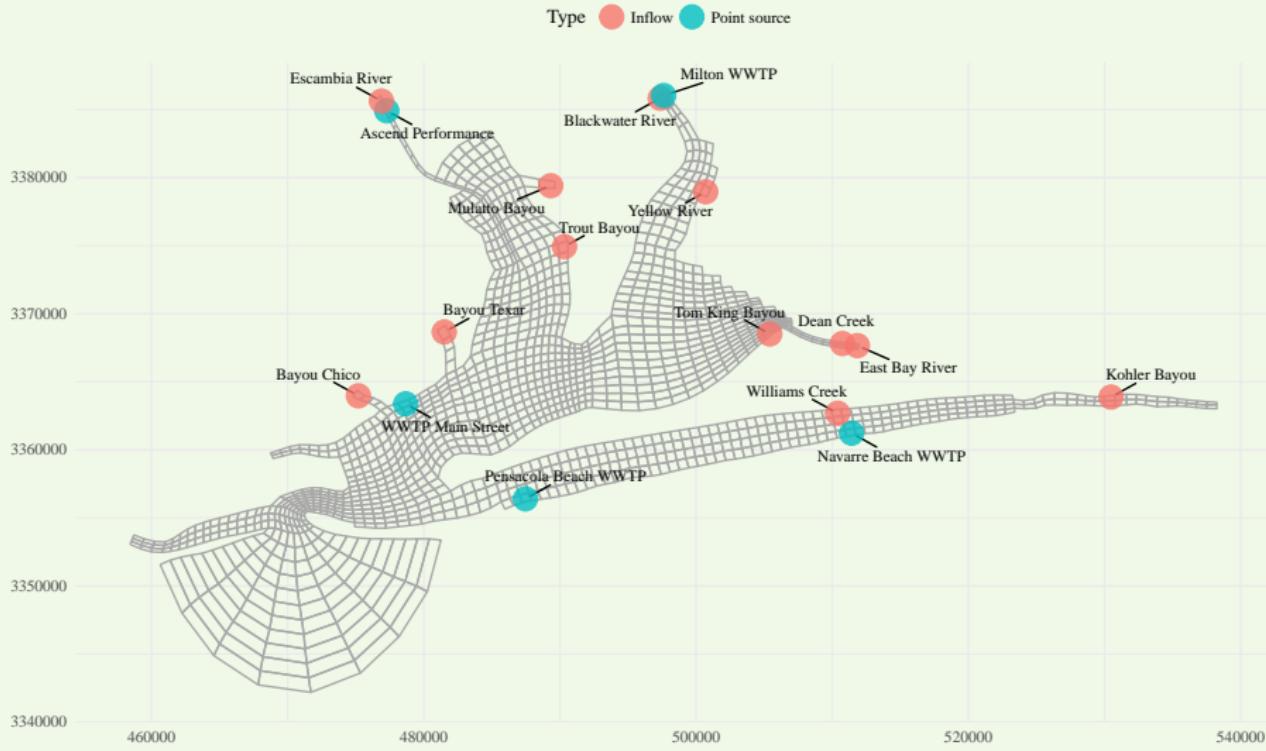
# The EPA experience

## 4.02B Nutrient Response and Recovery - PB model



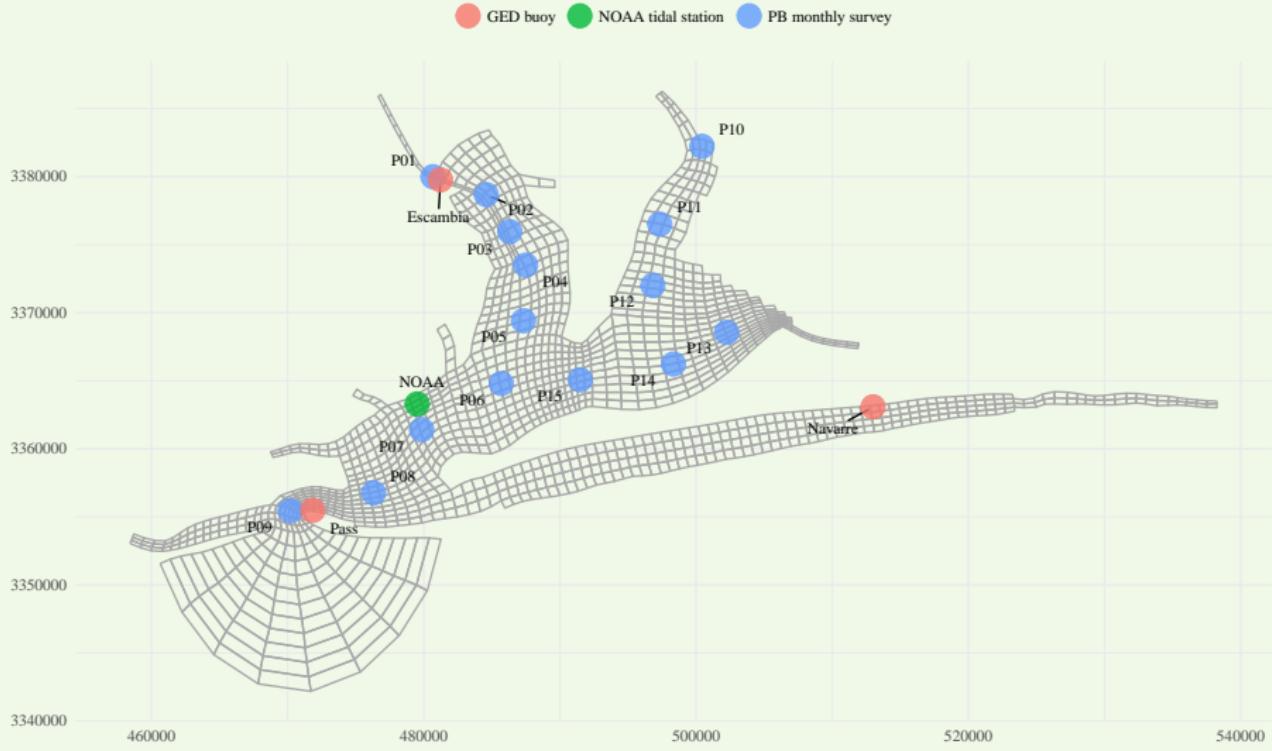
# The EPA experience

## 4.02B Nutrient Response and Recovery - PB model



# The EPA experience

## 4.02B Nutrient Response and Recovery - PB model



# The next chapter

*One beach destination to the next...*

*Pensacola \$*



*SoCal \$\$\$\$\$*



# The next chapter

## One car destination to the next...

Pensacola 🚗



SoCal 🚗🚗🚗🚗



# The next chapter



*A joint powers authority that works to develop a scientific foundation for informed water quality management in Southern California*

## Commission members:

- California State Water Resources Control Board
- USEPA, Region IX
- California Regional Water Quality Control Boards
- City of LA, San Diego
- LA/Orange County Sanitation Districts
- Ventura County Watershed Protection District
- LA County Flood Control District
- Orange County Public Works
- County of San Diego

# The next chapter



*A joint powers authority that works to develop a scientific foundation for informed water quality management in Southern California*

Six science depts:

- Toxicology
- Chemistry
- Biogeochemistry
- *Biology*
- Microbiology
- Information Management & Analysis

Research areas:

- Bioassessment
- Ecohydrology
- Eutrophication
- Climate change
- Sediment quality
- Contaminants of emerging concern
- Microbial water quality
- Regional monitoring
- Information technology and visualization

# The next chapter



*A joint powers authority that works to develop a scientific foundation for informed water quality management in Southern California*



## Final thoughts

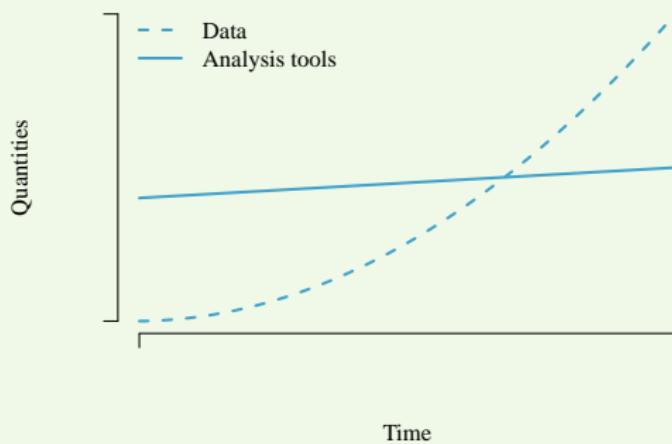
***The good news:*** We are getting better at collecting information - standardized, automated, increased coverage, real-time/continuous

***The bad news:*** Our ability to use this information has not kept pace with availability!

## Final thoughts

***The good news:*** We are getting better at collecting information - standardized, automated, increased coverage, real-time/continuous

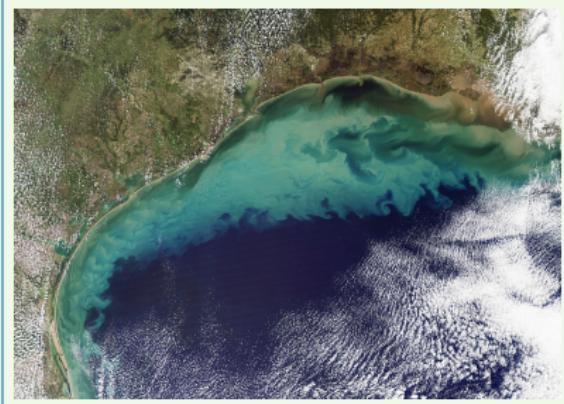
***The bad news:*** Our ability to use this information has not kept pace with availability!



# Final thoughts

## *Open Science for Synthesis: Gulf Research Program*

July 10 - July 28, 2017  
NCEAS, Santa Barbara, CA



# Final thoughts

## *Open Science for Synthesis: Gulf Research Program*

July 10 - July 28, 2017  
NCEAS, Santa Barbara, CA



<https://nceas.github.io/oss-2017/lessons.html>

- Collaboration modes and technologies, virtual collaboration
- Data management, preservation, and sharing
- Data manipulation, integration, and exploration
- Scientific workflows and reproducible research
- Programming using agile and sustainable software practices
- Data analysis and modeling
- Communicating results to broad communities

# Final thoughts

## *Open Science for Synthesis: Gulf Research Program*

July 10 - July 28, 2017  
NCEAS, Santa Barbara, CA



***Reproducible Science*** is transparent, automated, archived (provenance), and shared. It's also about modularity - one task, one component of the workflow.

Some bare necessities:

- Use the command line and learn to code
- Use version control
- Use community standards
- Use an archived data repository

# Final thoughts



*Man[/Woman] is condemned to be free; because once thrown into the world, he[/she] is responsible for everything he[/she] does.*

– J. P. Sartre

# Sincere thank-yous



Chengfeng Le, Leah Oliver, John Gazoo, James Hagy, Sandy Raimando, Darrin Dantin, Brandon Jarvis, John McCauley, Steven Jarrard, Peggy Rogers, Bernice Betts, David Bedick, Laura Enzor, Alex Almario, John Rogers, Brad Blackwell, Morgan Wilming, Marilynn Hoglund, Brian Plummer, Jim Harvey, Dragoslav Marcovich, Justin Bousquin, Katelyn Houghton, Leah Oliver, Marc Weber, George Craven, Leah Sharpe, Chloe Jackson, Joe James, Janet Nestlerode, Deb Vivian, Deb Santavy, Bill Benson, Jeanne Scott, Clay Peacher, Candice Lavelle, Ryan Heffernan, Jessica Lisa, Nancy Reeves, Rich Devereux, Diane Yates, Melissa Overton, Stephanie Friedman, Kyle Buck, Christina Horstmann, Lisa Lowe, Elizabeth George, Carl Litzinger, Matt Harwell, Susan Yee, Vic Camargo, Mike McManus, Jessica Aukamp, Michael Murrell, Elizabeth Paulukonis, Tripp Boone, John Lehrter, Sehan Lee, Ryan Boylan, Mace Barron, Ally Duffy, Yongshan Wan, Alice Watts, Bill Fisher, Paul Soderlind, Rick Greene, Jeff Hollister

# Sincere thank-yous



# References I

- Beck MW, Hagy III JD. 2015.  
**Adaptation of a weighted regression approach to evaluate water quality trends in an estuary.**  
Environmental Modelling and Assessment, 20(6):637–655.
- Beck MW, Hagy III JD, Murrell MC. 2015.  
**Improving estimates of ecosystem metabolism by reducing effects of tidal advection on dissolved oxygen time series.**  
Limnology and Oceanography: Methods, 13(12):731–745.
- Beck MW, Murphy RR. 2017.  
**Numerical and qualitative contrasts of two statistical models for water quality change in tidal waters.**  
Journal of the American Water Resources Association, 53(1):197–219.
- Beck MW, Vondracek B, Hatch LK. 2013.  
**Environmental clustering of lakes to evaluate performance of a macrophyte index of biotic integrity.**  
Aquatic Botany, 108:16–25.
- Beck MW, Wilson BN, Vondracek B, Hatch LK. 2014.  
**Application of neural networks to quantify the utility of indices of biotic integrity for biological monitoring.**  
Ecological Indicators, 45:195–208.
- Caffrey JM, Murrell MC, Amacker KS, Harper J, Phipps S, Woodrey M. 2013.  
**Seasonal and inter-annual patterns in primary production, respiration and net ecosystem metabolism in 3 estuaries in the northeast Gulf of Mexico.**  
Estuaries and Coasts, 37(1):222–241.

# References II

Levins R. 1966.

The strategy of model building in population biology.  
American Scientist, 54(4):421–431.

Odum HT. 1956.

Primary production in flowing waters.  
Limnology and Oceanography, 1(2):102–117.

Soetaert K, Petzoldt T. 2010.

Inverse modelling, sensitivity, and Monte Carlo analysis in R using package FME.  
Journal of Statistical Software, 33(3):1–28.

TBEP (Tampa Bay Estuary Program). 2011.

Tampa Bay Water Atlas.

<http://www.tampabay.wateratlas.usf.edu/>. (Accessed October, 2013).