Update on the 4-dimensional interpolator progress

Rebecca Murphy (UMCES) and Peter Tango (USGS)
Bay Oxygen Research Large Group
Feb. 12, 2024

Key input on presentation from:
Elgin Perry (statistics consultant) and Jon Harcum (Tetra Tech)
Breck Sullivan (USGS) and August Goldfischer (CRC)

Presentation outline

- Reminder – Why a 4D interpolator?
- Data sources being used (more from Jay Lazar in next presentation)
- Daily DO interpolation (Rebecca)
- Hourly DO evaluation (Rebecca)
- Thoughts on feeding into criteria evaluation (Peter)
- Documentation (Peter)

Why a 4D interpolator?

- USEPA (2003) published Ambient Water Quality Criteria for Chesapeake Bay, need for criteria assessment protocols.

- **2007 STAC Workshop: Assessing the feasibility of developing a four-dimensional (4-D) interpolator for use in impaired waters listing assessment**

Why is the Chesapeake Bay Program interested in 4d interpolation?

  - *To allow combining and integrating measurements from numerous disparate datasets*
  - *To generate a more complete interpolation of available data in space and time.*
  - *To improve the ability to evaluate water quality for the 303d listing process.*

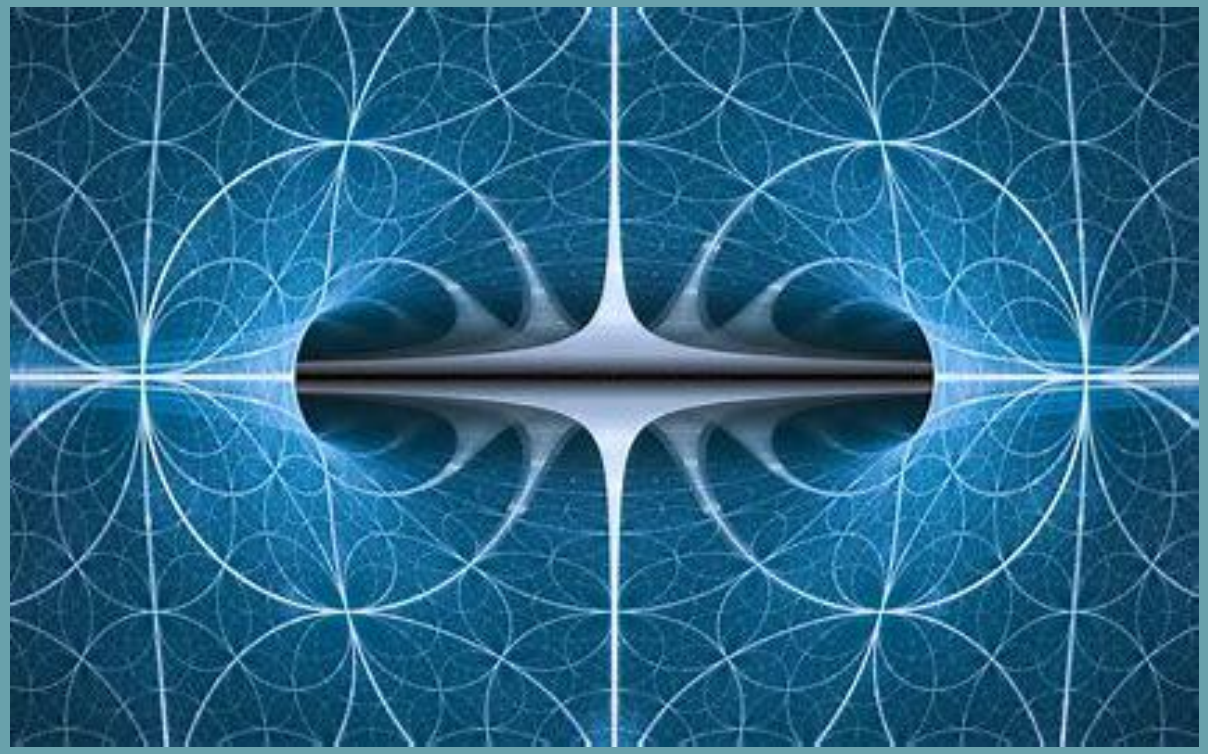
Curriero et al. 2008 STAC Workshop Report

2007 STAC Workshop consensus

- Sampling frequency (biweekly to monthly) is insufficient
- Spatial resolution of the existing Chesapeake Bay datasets is insufficient
  - *for successful extrapolation to four dimensions.*

"However, there is an on-going effort among Chesapeake Bay partners to acquire funding to deploy continuous monitoring buoys, which are equipped with vertical profilers in deep water areas of the Chesapeake Bay and tidal tributaries. If these efforts succeed, then the shortcomings of existing datasets will be greatly alleviated."

Curriero et al. 2008 STAC Workshop Report



17 YEARS LATER…WHERE ARE WE TODAY?

Welcome to the Chesapeake Bay 4D water quality interpolator development program!

Bay Oxygen Research Group – Development Team

- Coordinators - Rebecca Murphy (UMCES) and Peter Tango (USGS)
- STAR Staffer - August Goldfischer (CRC)
- Development to-date - Elgin Perry (statistician); Jon Harcum and Erik Leppo (Tetra Tech); Angie Wei and Rebecca Murphy (UMCES/CBP)
- Advisory Team
  - Richard Tian (UMCES), Gary Shenk (USGS), Isabella Bertani (UMCES), Jim Hagy (EPA), Breck Sullivan (USGS), Kaylyn Gootman (EPA)
- ORISE Fellow – Wes Slaughter, U of MD Ph.D. candidate

4-D interpolator development timeline

Draft January 2024

Priority categories for 2024 are in red

Calendar Year	2022				2023				2024				2025				2026				2027			
Calendar Quarter	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec	Q1 Jan-Mar	Q2 Apr-Jun	Q3 Jul-Sep	Q4 Oct-Dec
Project Year	Year 1				Year 2				Year 3				Year 4				Year 5				Year 6			
1. Development-daily estimates	■	■	■	■	■	■	■	■	■	■	■													
2. Develoment-hourly estimates					■	■	■	■	■	■	■	■												
3. Development - shallow water							■	■	■	■	■	■	■	■	■									
4. Development - GIS tasks	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■							
5. Development -combined daily & hourly								■	■	■	■	■	■											
6. Development-criteria evaluation								■	■	■	■	■	■	■	■	■								
7. Software							■	■	■	■	■	■	■	■	■	■								
8. Documenting	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■				
9. Training													■	■	■	■								
10. Year of Review																	■	■	■	■				
11. Operational																					■	■	■	■

Future meeting considerations

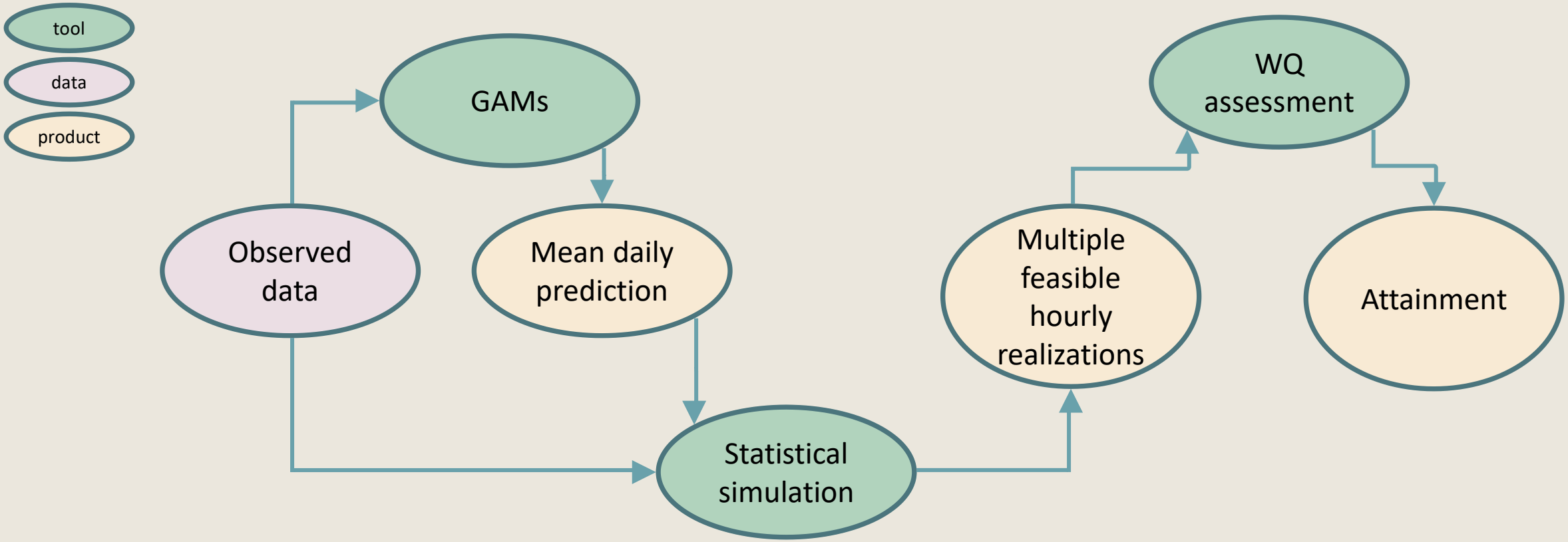
Through 2024-2025 development years:

1. **Bay Oxygen Research Group:** This large group of developers, stakeholders, future users, researchers
   - *We will meet approximately every 3 months*

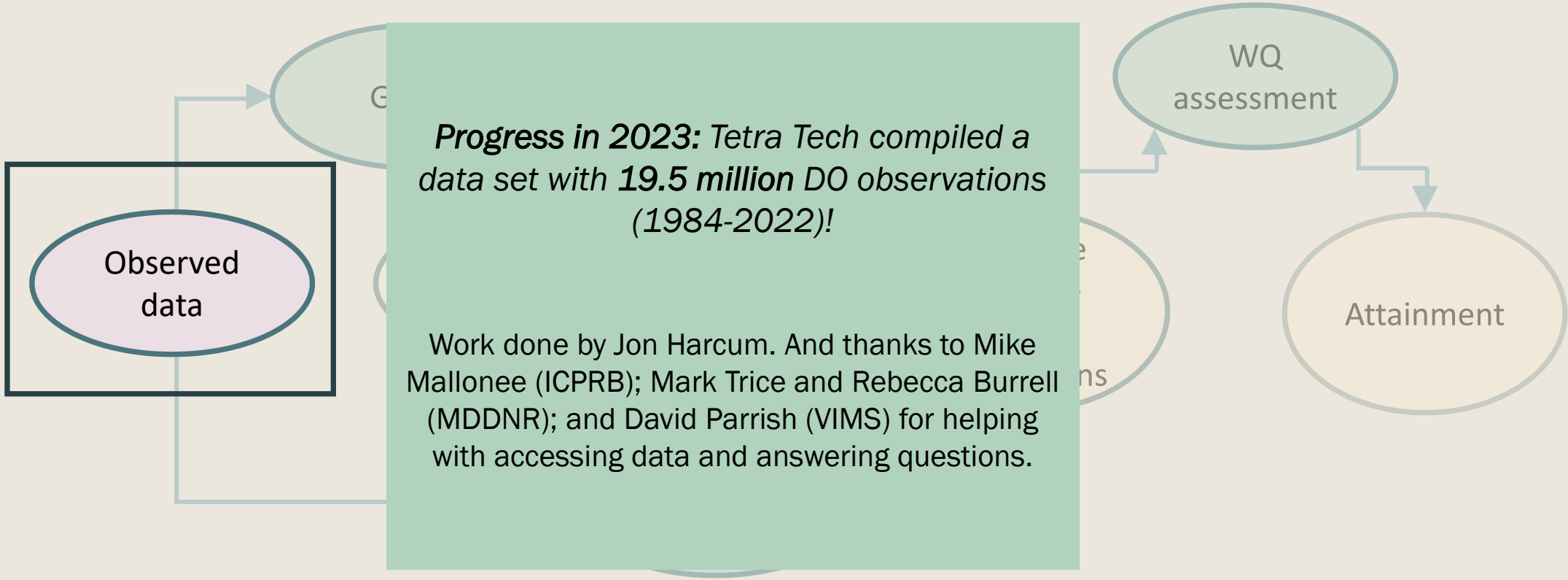
2. **Smaller BORG development group** –
   - *meets monthly 3rd Monday 12:00-12:50*
   - *Currently: CBP staff, contractors, EPA researchers*
   - *We'd like any future users to join the monthly meetings who want to know more details about the technical development*

Based on what you hear today, let us know if you or someone in your group should be on the Development Team invite. We'll send a reminder with the minutes.

WQ Assessment with 4D interpolator



Full use of the data

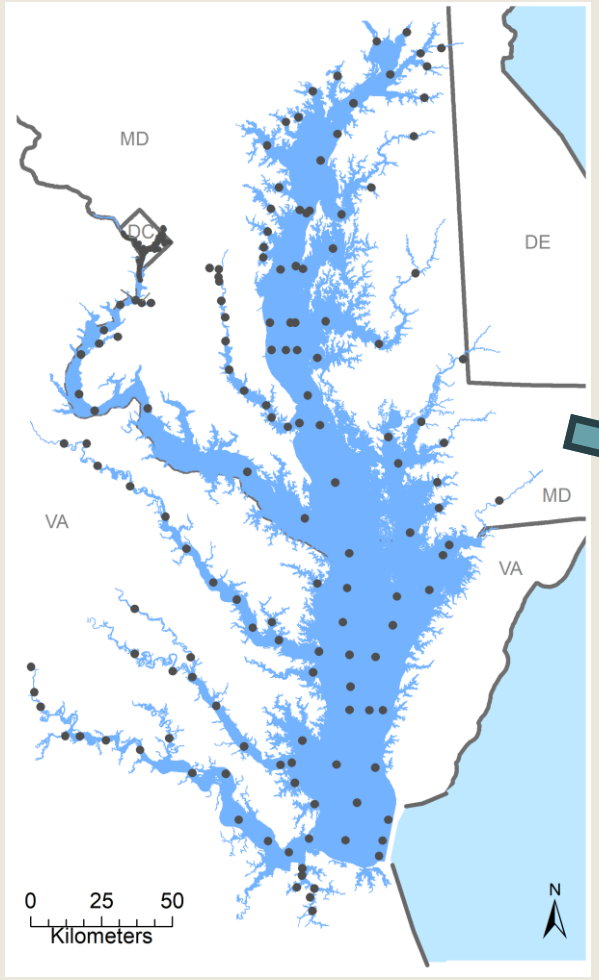


Progress in 2023: *Tetra Tech compiled a data set with* ***19.5 million*** *DO observations (1984-2022)!*

Work done by Jon Harcum. And thanks to Mike Mallonee (ICPRB); Mark Trice and Rebecca Burrell (MDDNR); and David Parrish (VIMS) for helping with accessing data and answering questions.

Full use of the data

Bi-weekly long-term sampling
(DOEE, MDDNR, VADEQ, CBP)



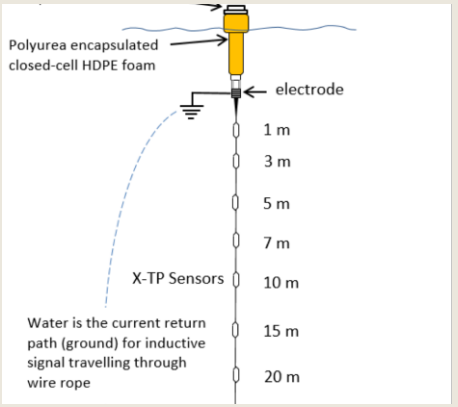
Shallow water continuous monitoring
(MDDNR and VECOS)

From https://eyesonthebay.dnr.maryland.gov/

From http://vecos.vims.edu/

Observed data

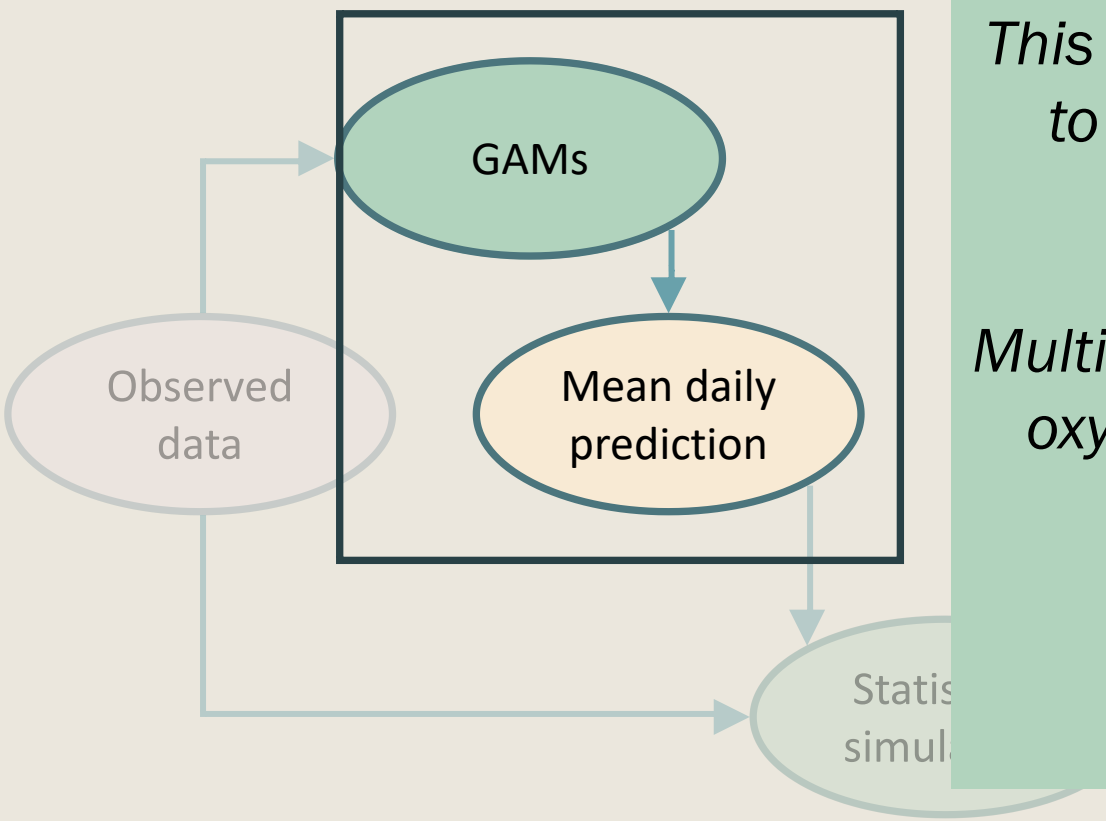
New continuous vertical arrays (NOAA & CBP)



https://www.chesapeakebay.net/who/group/hypoxia-collaborative-team

And more for validation & testing: Citizen science, data collected with fisheries studies, and research data sets

Generalized additive model (GAM):

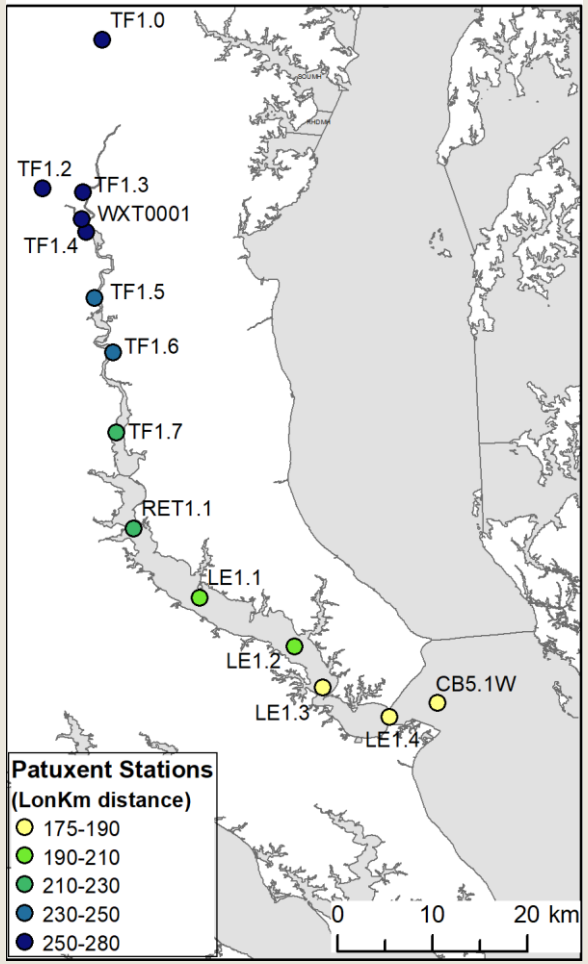


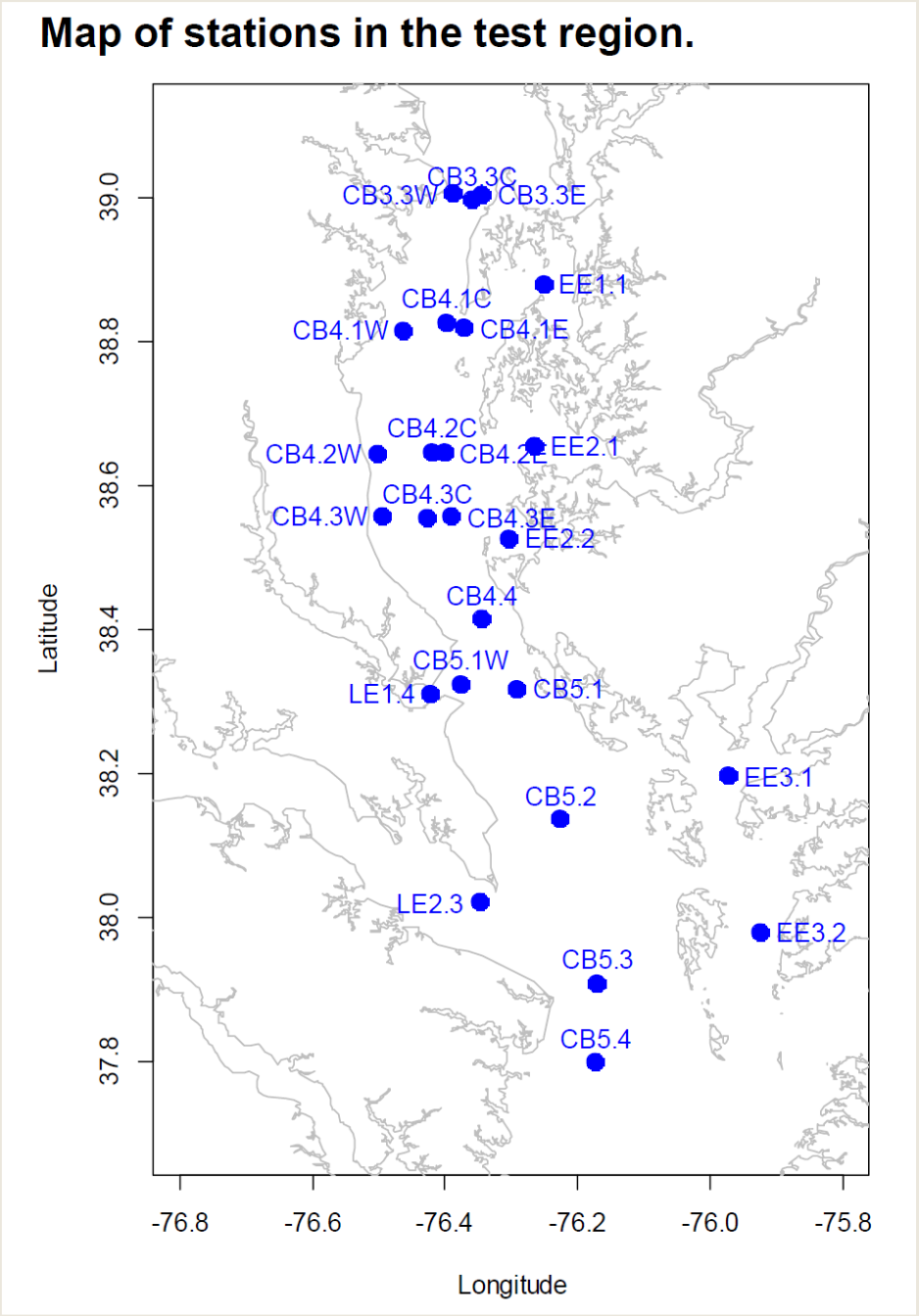
This is a statistical approach that uses data to generate a smooth function of DO in space and time.

Multiple fitted GAMs will be used to estimate oxygen daily throughout the tidal waters:

DO ~ smooth function(date, x, y, z)

Daily mean:
Test applications

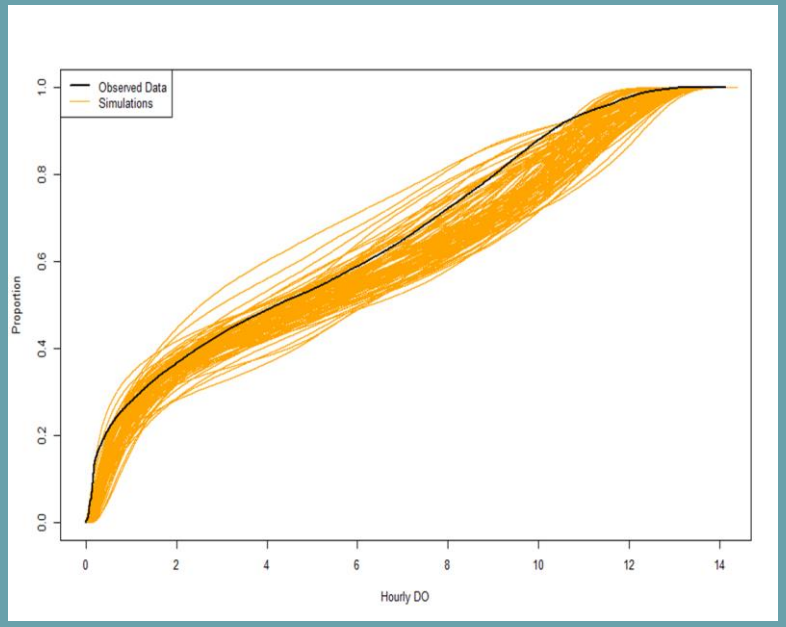




Daily mean: Current work

Transforming DO

- We have challenges with both bounded DO values and a high frequency of low DO.
- Result is that a normal distribution assumption being a poor choice.
- Elgin Perry has been working on an approach ("beta-logit") to address these.



Example analysis: CDF of 1 station's bottom data superimposed on CDFs of 100 simulations using resampling with Beta-Logit Transform

Bay-wide scale-up

Phase 1: Scale-up > Framework > Scale up Testing

Scale up
- Sub-estuary
- `by` term

'do ~ s(date_d, k = 20, by = reg)')

cbseg_92	cb_303d_segment	cb4d_model	add_data	cb4d_by2	cb4d_by3	cb4d_by4
CB4MH	Middle Central Chesapeake Bay	CB1_3	TRUE			
CB3MH	Upper Central Chesapeake Bay	CB1_3	FALSE			
CB2OH	Upper Chesapeake Bay	CB1_3	FALSE			
CB1TF	Northern Chesapeake Bay	CB1_3	FALSE			
MAGMH	Magothy River	CB1_3	FALSE	West	West	MAG
PATMH	Patapsco River	CB1_3	FALSE	West	West	PAT

Phase 1: Data
- 1984-2022
- 844 stations
- 19.5M obs.

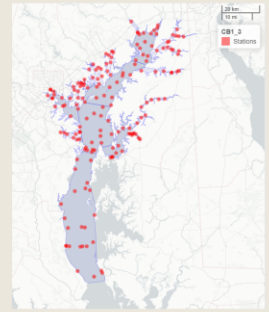
Filter
- Sub-estuary
- Date range

Scale up
- GAM model

```
do ~ s(date_d, k = 20, by = reg) +                                  #_002*
  s(doy, bs = "cc", by = reg) +                                     #_003*
  s(depth, k = 4, by = reg) +
  s(wb_lon_km, k = 4, by = reg) +
  s(wb_lat_km, k = 4, by = reg) +
  s(depth_b, k = 4, by = reg) +
  ti(wb_lat_km, depth, wb_lon_km, k = c(3, 3, 3), by = reg) +       #_004*
  ti(depth, depth_b, k = c(3, 3), by = reg) +                       #_005*
  ti(depth, date_d, by = reg) +
  ti(wb_lon_km, date_d, by = reg) +
  ti(wb_lat_km, date_d, by = reg) +
  ti(depth_b, date_d, by = reg) +
  ti(depth, doy, bs = c("tp", "cc"), by = reg) +
  ti(wb_lon_km, doy, bs = c("tp", "cc"), by = reg) +
  ti(wb_lat_km, doy, bs = c("tp", "cc"), by = reg) +
  ti(depth_b, doy, bs = c("tp", "cc"), by = reg) +
  ti(date_d, doy, bs = c("tp", "cc"), by = reg)
```

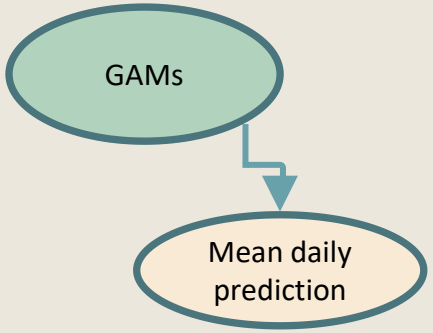
#: 2023_10_23

CB1_3

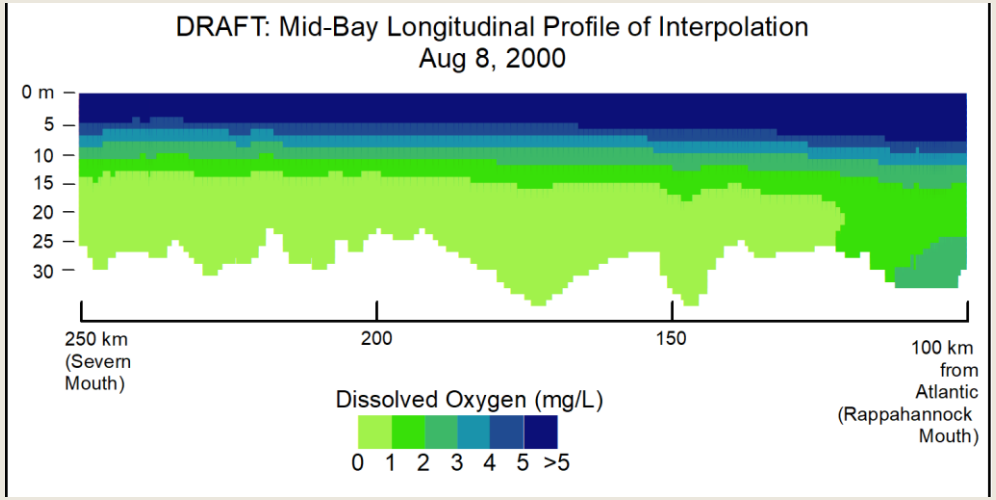


- Basic code has been built in R to apply GAM to each segment (Jon Harcum, Tetra Tech).
- Currently testing spatial and temporal options.
- Modifications will continue as we develop the method and link it to other components.

Where we are:



Example: GAM-based DO predictions along part of main channel



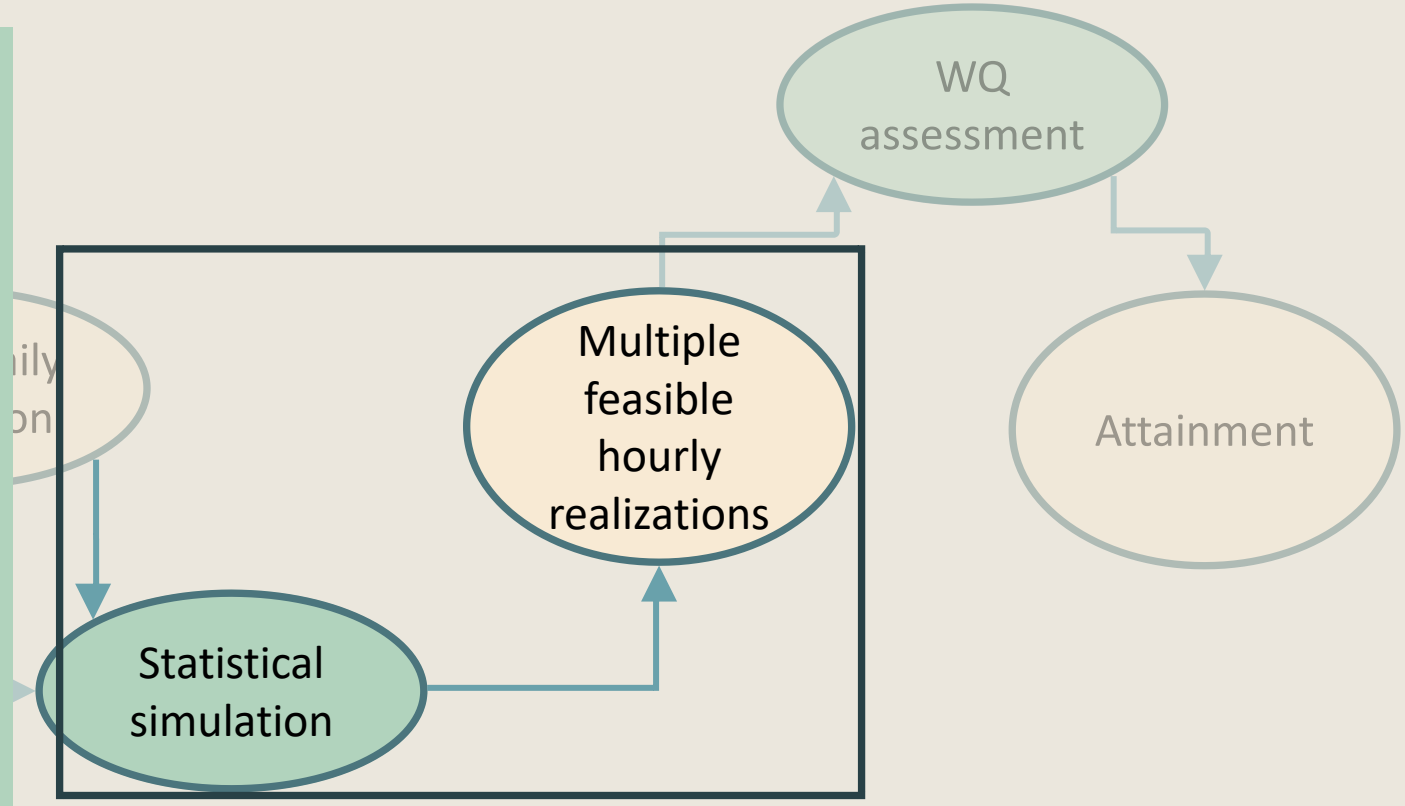
Status and schedule	Development item
✓	Pilot application to mid-bay
✓	Test and modify approach in Patuxent
Current work, Q1 2024	Identify appropriate statistical distribution for low DO
Current work, Q1 2024	Build structure for bay-wide implementation
Q2 2024	Test GAM approach on density/pycnocline
Q2 2024	Draft of bay-wide implementation
Q3 2024	Spatial validation of GAM estimates using additional data sets
Q3 2024	Develop approach for daily error estimates
Q4 2024 to Q4 2025	Continued updates as hourly approach is developed

Q1=Jan-Mar, Q2=Apr-Jun, Q3=Jul-Sep, Q4=Oct-Dec

Hourly prediction

Involves evaluating all existing continuous monitoring DO data for within-day variability.

And then applying those patterns in a simulation to make hourly variability estimates bay-wide.



Method development with high frequency data

✓

Have scanned through all common data from MDDNR and VECOS and recent NOAA vertical array data. Going to use this data to inform variability.

Work done by Erik Leppo and Jon Harcum at Tetra Tech.

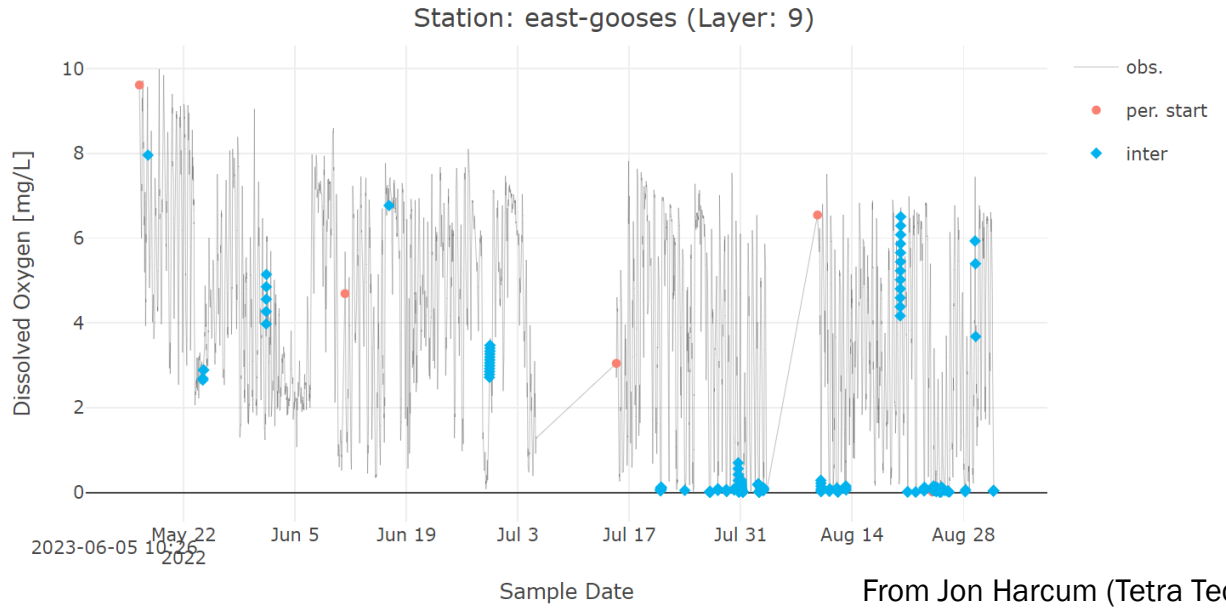
Example: Current processing technique from Tetra Tech team using East Goose's array in 2022 at 9m

3.10.2 Period Summary

Period Summary

period	per_date_time_first	time_diff	rec_num_first	rec_num_last	rec_num	per_date_time_last	per_length	per_keep	num_int	rec_freq
1	2022-05-16 11:00:00		1	3659	3659	2022-06-10 20:40:00	2194800s (~3.63 weeks)	TRUE	10	600s (~10 minutes)
2	2022-06-11 06:50:00	36600s (~10.17 hours)	3660	7123	3464	2022-07-05 08:00:00	2077800s (~3.44 weeks)	TRUE	13	600s (~10 minutes)
3	2022-07-15 09:10:00	868200s (~1.44 weeks)	7124	9842	2719	2022-08-03 06:10:00	1630800s (~2.7 weeks)	TRUE	98	600s (~10 minutes)
4	2022-08-09 15:50:00	553200s (~6.4 days)	9843	11897	2055	2022-08-23 22:10:00	1232400s (~2.04 weeks)	TRUE	57	600s (~10 minutes)
5	2022-08-24 02:30:00	15600s (~4.33 hours)	11898	12989	1092	2022-08-31 19:20:00	665400s (~1.1 weeks)	TRUE	45	600s (~10 minutes)

3.10.3 Final Values



From Jon Harcum (Tetra Tech)

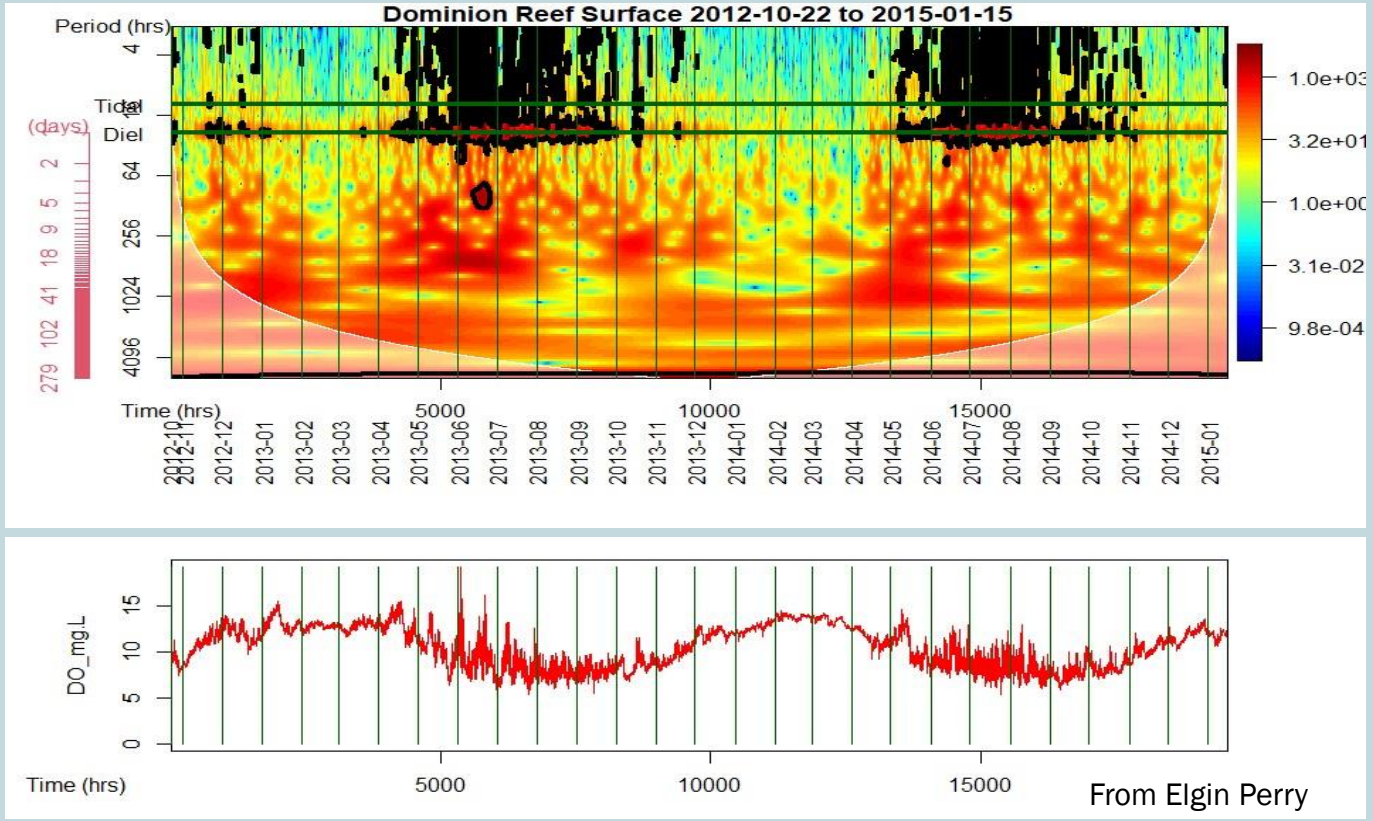
Method development with high frequency data

Conducted preliminary work with wavelet analysis on high frequency data and identifying sub-daily cycles.

Processing of the results is underway.

Concept worked on by Elgin Perry with analysis of all high frequency by Erik Leppo and Jon Harcum.

Example: Wavelet analysis of gap-filled data to identify cycles



Method development with high frequency data

Idea: Will fit a mathematical model to the sub-daily cycles observed in the data and use a statistical approach to account for the uncertainty in these estimates.

Development planned for 2024

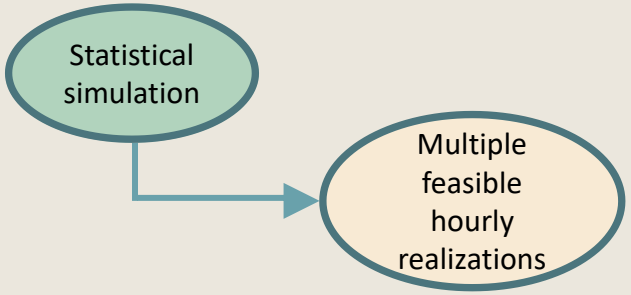
Example: Fourier analysis with just daily cycle to fit hourly DO (DO_h)

$$DO_h = lc * h + sc * sin\left(\frac{2\pi * h}{24}\right) + cc * cos\left(\frac{2\pi * h}{24}\right) + \tau_h$$

coefficients

h = hour 1:24

Where we are:



Example: High frequency data processing

3.10.2 Period Summary

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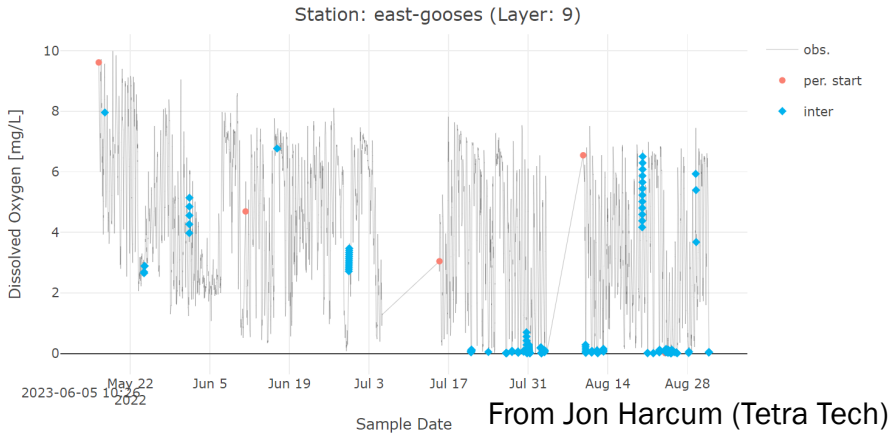


From Jon Harcum (Tetra Tech)

Status and schedule	Development item
✓	Investigate method for hourly prediction at 1 to 2 continuous monitoring stations
✓	Standardize continuous data processing
Current work, Q2 2024	Compare (and update) approach at additional continuous monitoring stations
Q3 2024	Investigate approach for predicting hourly DO
Q4 2024	Evaluate need for small scale spatial error term
Q4 2024	Implement approach for modeling hourly predictions
Q4 2024 to Q4 2025	Continued development and integration of daily & hourly tools

Q1=Jan-Mar, Q2=Apr-Jun, Q3=Jul-Sep, Q4=Oct-Dec

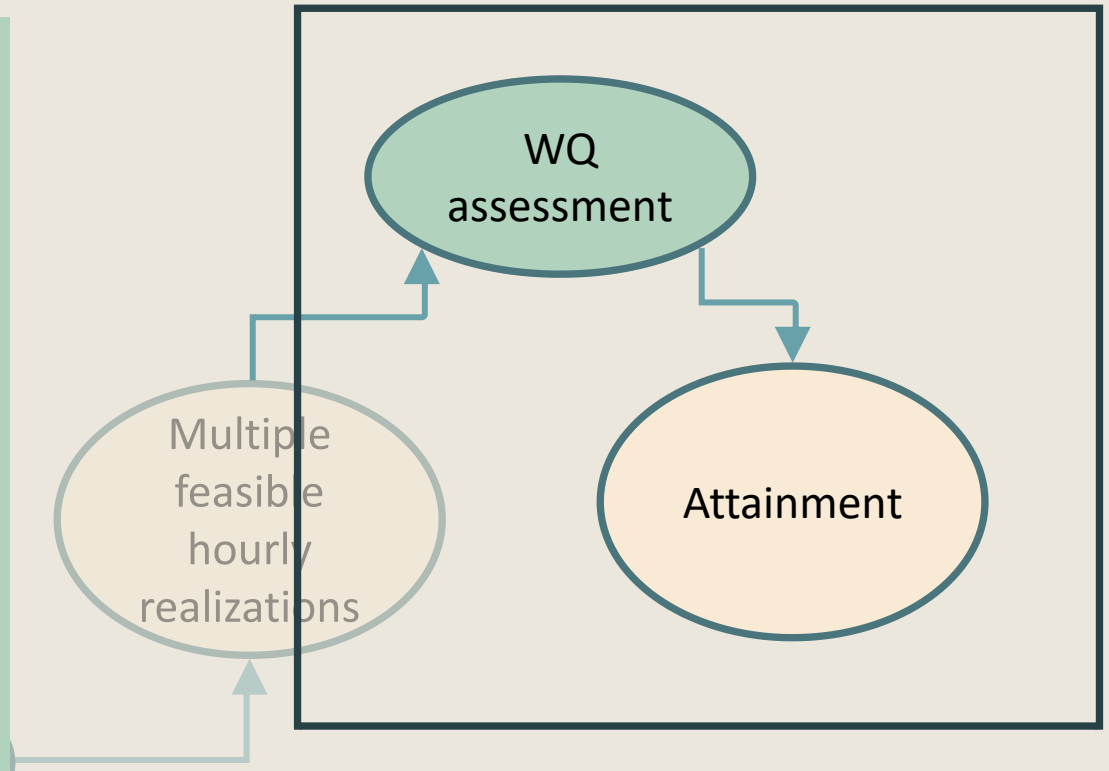
Link to WQ assessment

4d interpolator outputs will not be precise hourly DO estimates.

The goal is for them to provide a measure of segment impairment over the appropriate temporal and spatial scale for a criterion.

Timeline for development: ongoing through 2024-2025

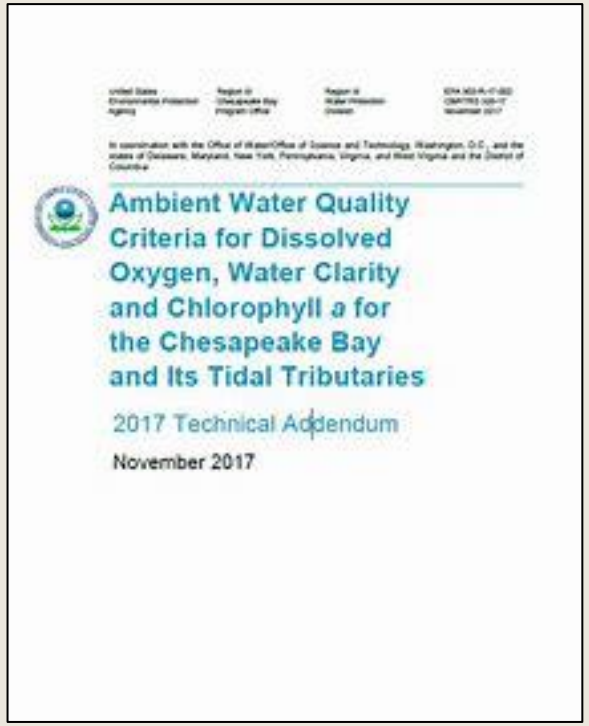
Decision protocols: CAP WG, Modeling WG, EPA



Documentation

- Creating a new EPA Technical Document supporting
  - *Dissolved oxygen chapters needed include*
    - Development underpinnings of the new 4D tool
    - Updates on dissolved oxygen assessment protocols

- Outline shared among team for review



Thank you!

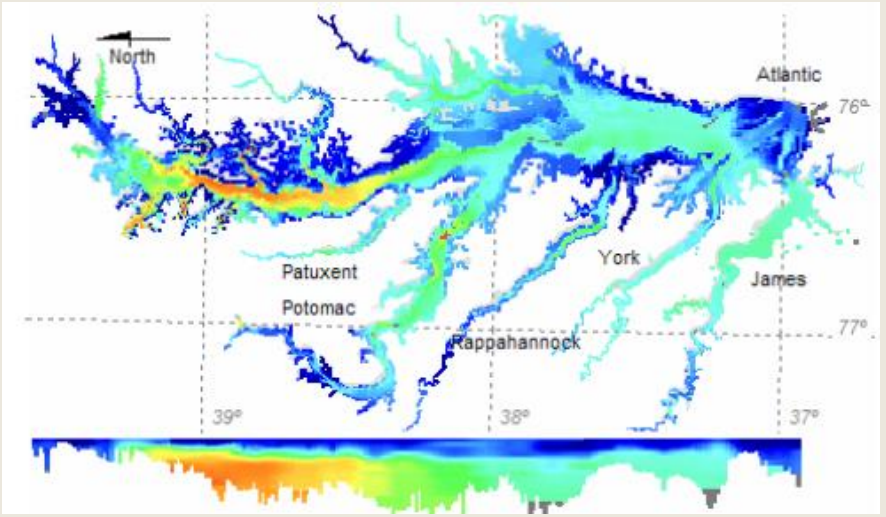
extras

Requirements for an Updated Chesapeake Bay Interpolator

- **New features:**
  - *Temporal and spatial interpolation of water quality parameters in Chesapeake Bay*
  - *Statistical estimates of uncertainty in the estimates*
  - *Reproduce the short-term variability in the data*
  - *Integrated vertical interpolation technique*
- **Features to retain and update:**
  - *Usability by partner analysts with automation for routine analyses*
  - *Visualization of the results*
  - *Analysis of dissolved oxygen, clarity, and chlorophyll a*
  - *Post-processing to identify regions for each designated use (DU)*
  - *Reasonable spatial extents for interpolation (e.g., not interpolating across land)*
  - *Incorporation of new data streams & types, as available*

Current interpolation

- Uses **inverse-distance weighting** of observations from long-term fixed stations, plus additional data as possible.
- **Temporal: snapshots,** generally using data collected within a week or two
- **Spatial:**
  - *Horizontal: Grid 1km x 1km in mainstem, finer (50m) in tribs*
  - *Vertically: Interpolation are done horizontally for every 1m in depth, and stacked to get 3d results*



VOL3d program output, Bahner 2006