Kriging-based Interpolation of Dissolved Oxygen in Chesapeake Bay

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CBP Tidal Monitoring and Analysis Workgroup Dissolved Oxygen Seminar

May 7, 2013

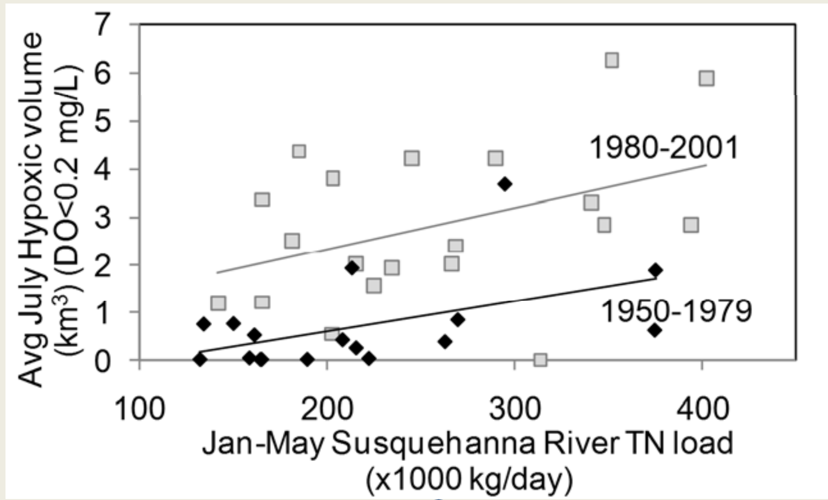
Guiding Questions/Outline

- What method(s) do you use for assessing DO?
- Why did you choose that methodology?
- What have you found drives DO patterns in the Bay?
- What lessons have you learned that we should consider as we move forward?

Outline

- What method(s) do you use for assessing DO?
- Why did you choose that methodology?
  - For analysis of the relationship between hypoxic volume and nitrogen loads in Chesapeake Bay
- What have you found drives DO patterns in the Bay?
- What lessons have you learned that we should consider as we move forward?

Hypoxia: Shift in relation to nutrient loads?



Based on: Hagy et al. (2004) *Estuaries* 27: 634-658. and Kemp et al. (2005) *Marine Ecology Progress Series* 303: 1-29.

investigate

CBEO
Chesapeake Bay Environmental Observatory

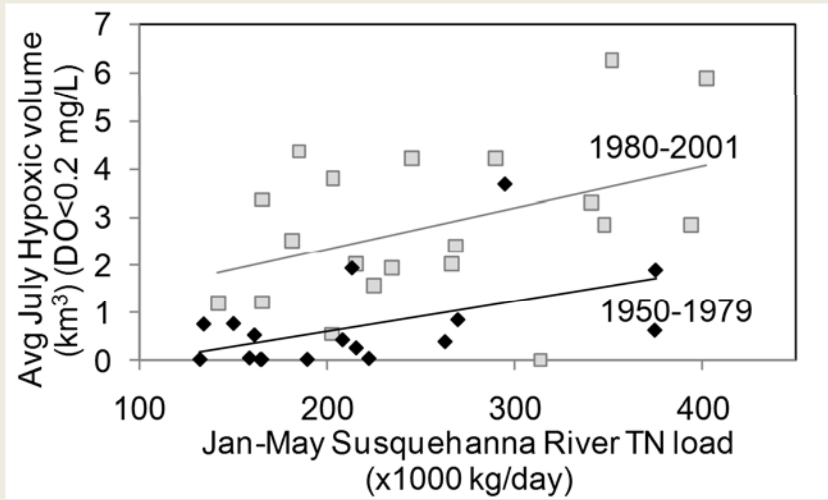
CBEO website: http://cbeo.communitymodeling.org

Data Sets
CBP data
USGS River Monitoring
Historic Chesapeake Bay Institute data
Model outputs, etc…

+

New Tools/ Methods

Hypoxia: Shift in relation to nutrient loads?



Based on: Hagy et al. (2004) *Estuaries* 27: 634-658. and Kemp et al. (2005) *Marine Ecology Progress Series* 303: 1-29.

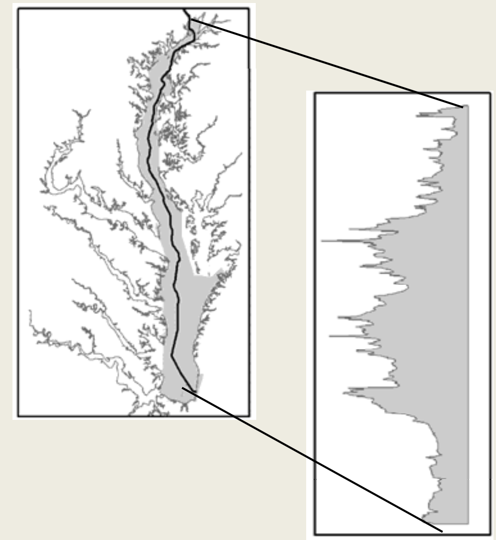
Hypotheses investigated by CBEO team

- Is the shift an artifact of the interpolation method used?
- Has there been a change in the stratification of the bay?
- Has there been an increase in other nutrient loads besides TN from the Susquehanna River?
- Could enhanced nutrient recycling from the sediment account for the difference?

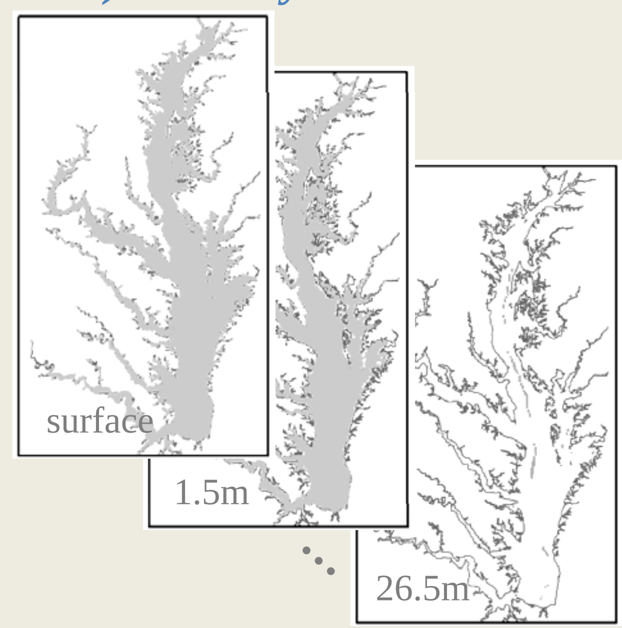
Outline

- What method(s) do you use for assessing DO?
  - DO analysis: Hypoxic volume
  - Spatial interpolation: Kriging
  - Extent:
    - Main-stem only
    - Full-bay
- Why did you choose that methodology?
- What have you found drives DO patterns in the Bay?
- What lessons have you learned that we should consider as we move forward?

1) Main-stem method



2) Full-bay method



Spatial Interpolation: Different methods

General: Weighted average prediction

$$\hat{Y}(s_0) = \sum_{i=1}^{n} w(s_i) Y(s_i)$$

s_0 = location (x,y) to predict at

s_i = different x,y location with measured value

$\hat{Y}(s_0)$ = value predicted at location s_0

$Y(s_i)$ = value measured at location s_i

$w(s_i)$ = weight assigned to measured value at s_i

Non-statistical

Statistical

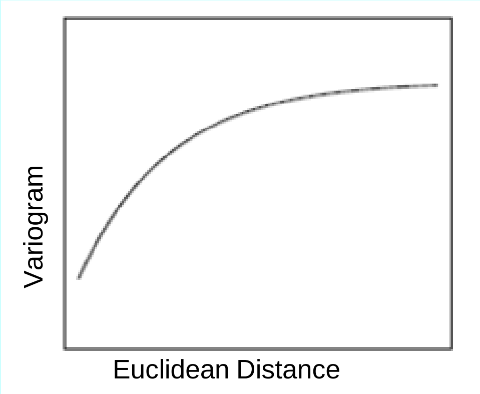
Inverse distance weighting (IDW) squared predictor weights

$$w(s_i) = \frac{1/d_i^2}{\sum_{j=1}^{n} \left(1/d_j^2\right)}$$

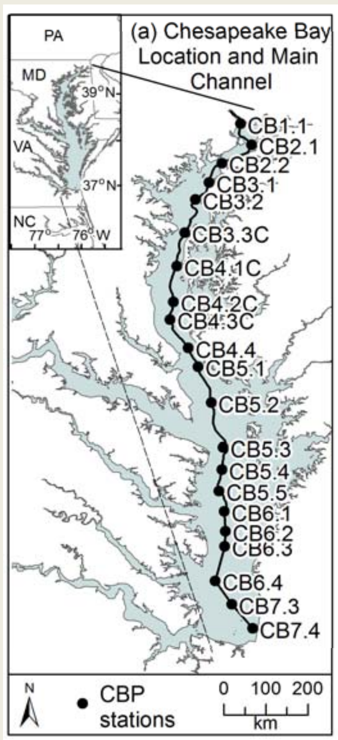
d_i = distance between s_o and location s_i

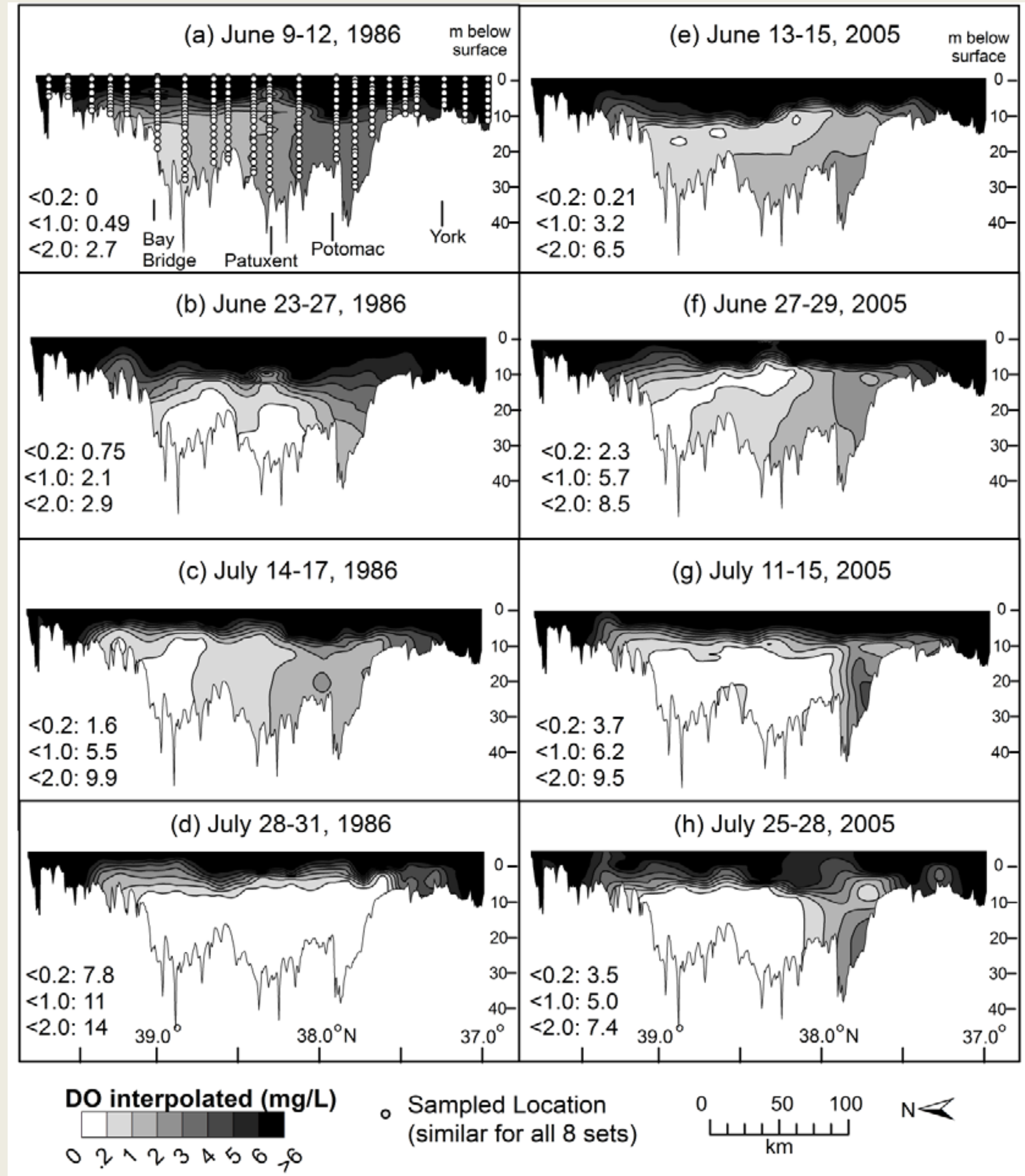
Kriging predictor weights

$w(s_i)$ is dependent on the spatial relationship between the observed data, as quantified with a variogram



Method 1:
Main stem DO

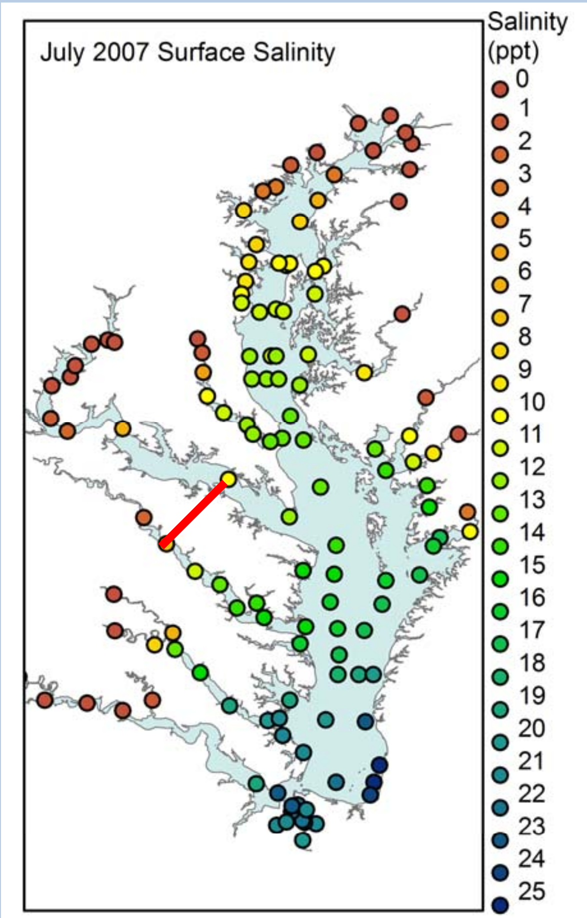




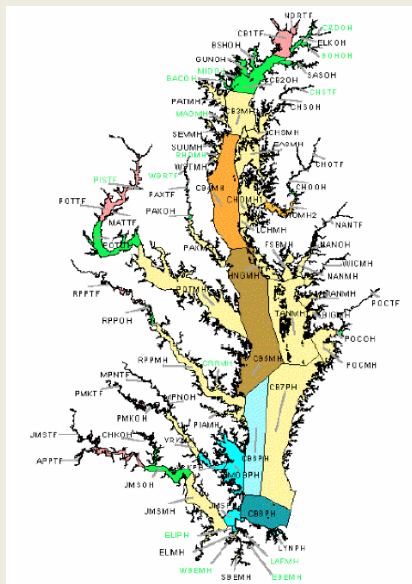
Murphy, Kemp, and Ball . 2011.
Estuaries and Coasts 34:1293-1309.

Method 2: Full-bay method

Challenge for interpolation in estuaries: Shape

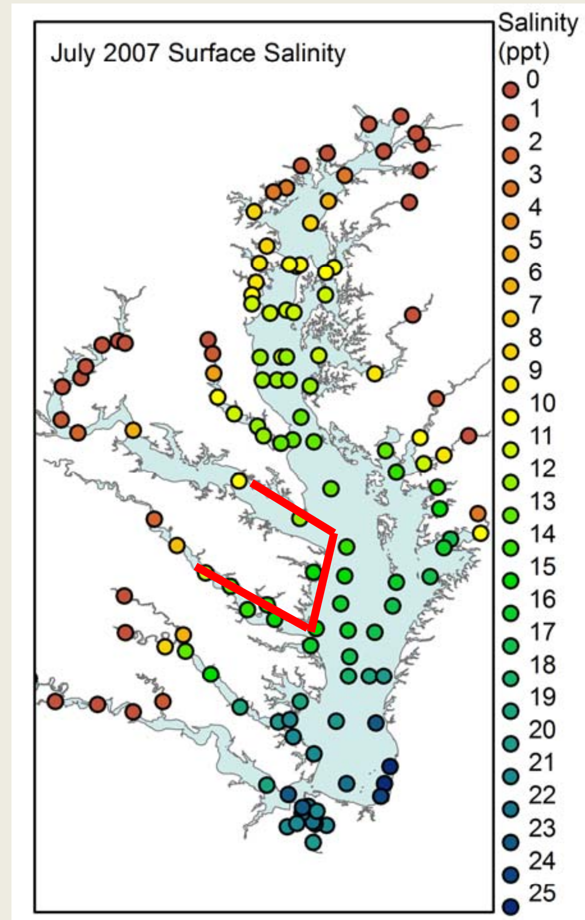


Solution 1: Segmentation



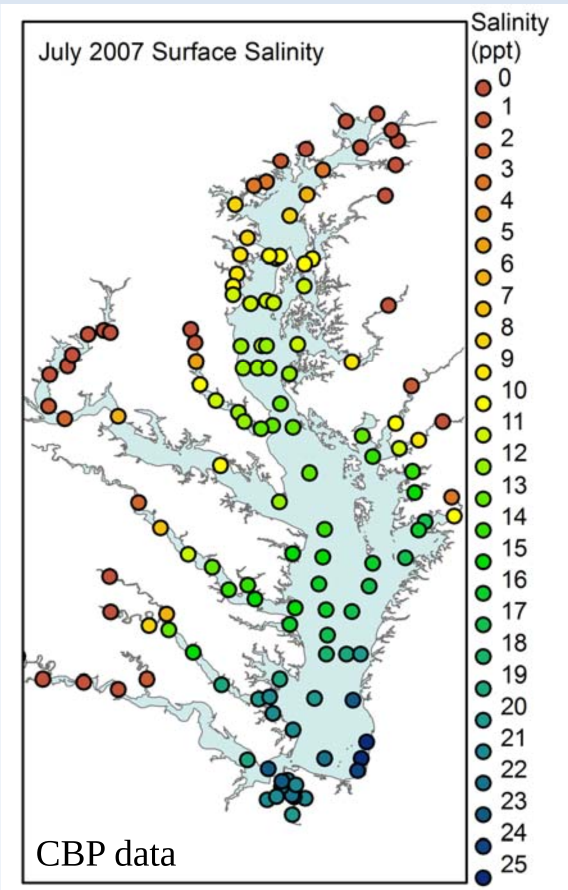
Chesapeake Bay Program 1998 segmentation design.

Solution 2: Water distance

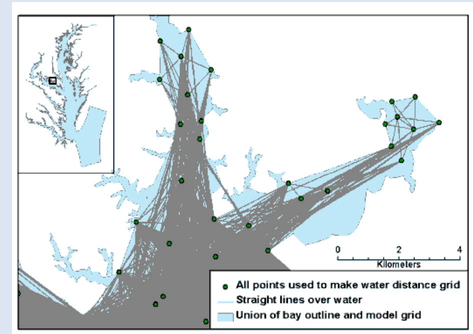


Method 2: Full-bay method – surface only

Use all data below fall-line in Bay



Compute “water distance” between all samples and points on a prediction grid

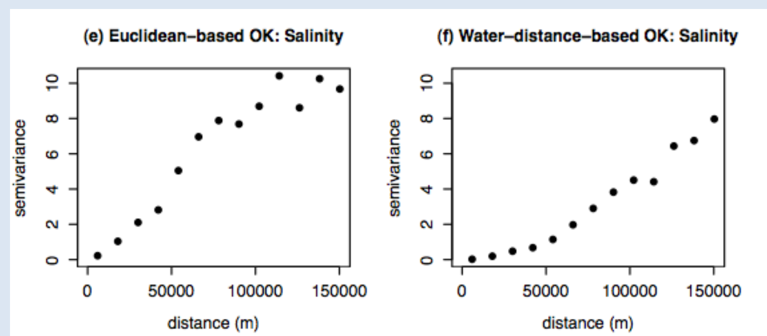


Water distances computed by Eric Perlman

Transform matrix of water distances into Euclidean distances with multi-dimensional scaling

$$\begin{bmatrix} d_{11} & \dots & d_{n1} \\ \dots & \dots & \dots \\ d_{1n} & \dots & d_{nn} \end{bmatrix}$$

Use transformed distances to compute variograms and perform kriging

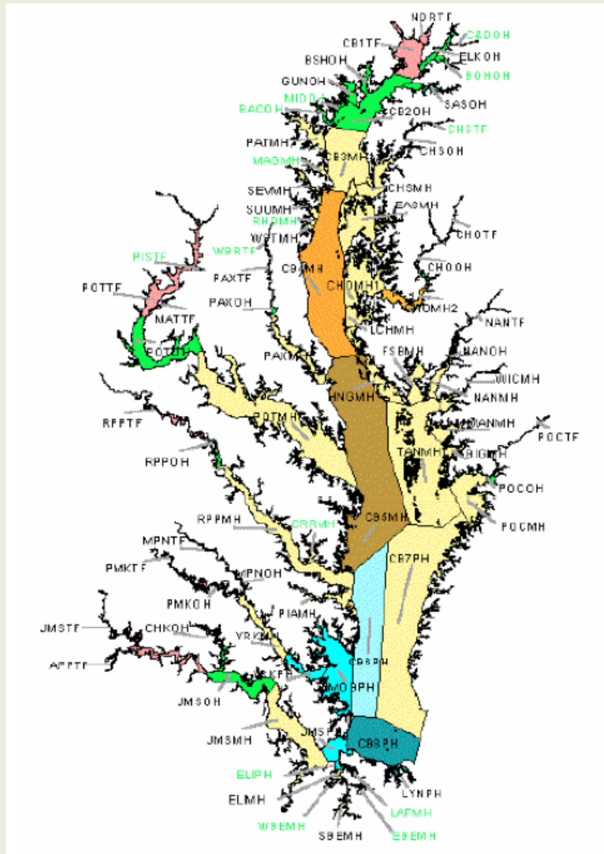


Compare to two other methods

Perform comparisons for:

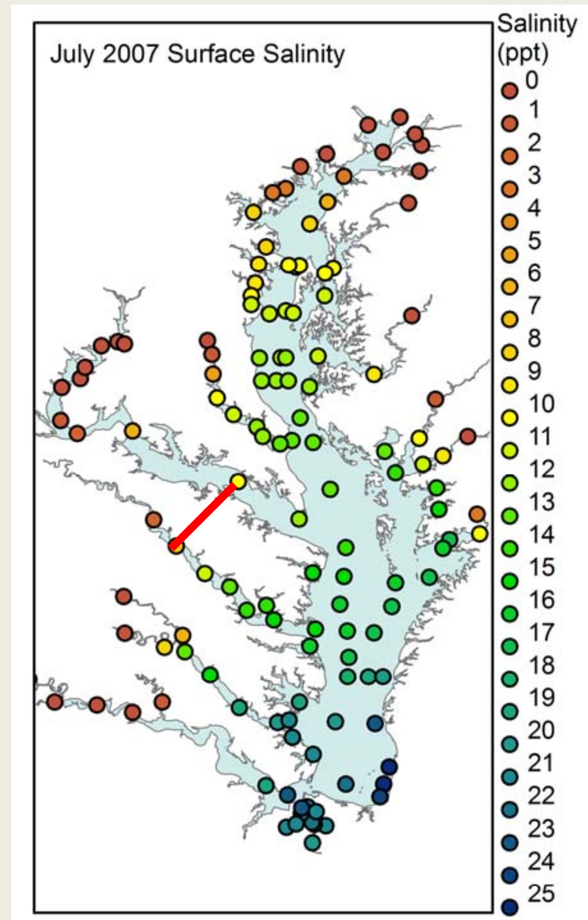
- Seven parameters in surface layer
- Multiple datasets in 2007 and 2008

a) Segmented IDW



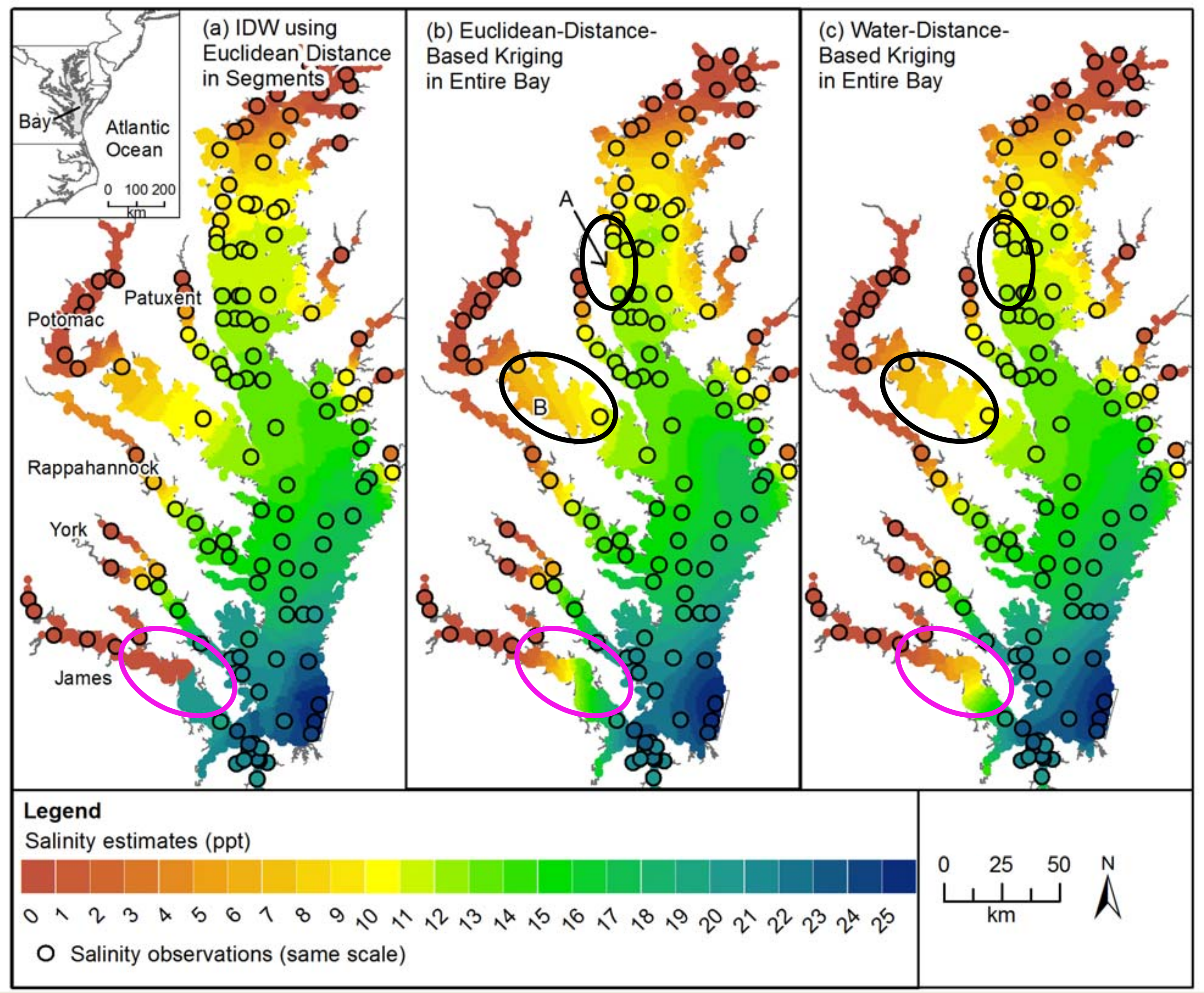
Chesapeake Bay Program 1998 segmentation design.

b) Kriging with Euclidean distance



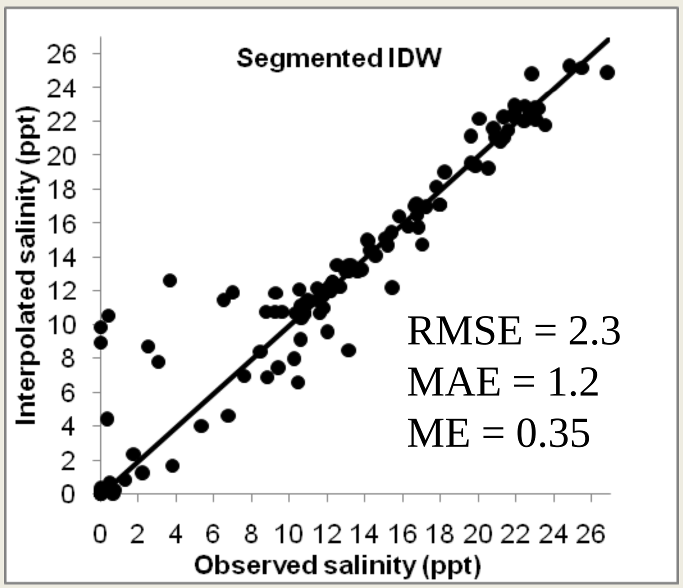
Surface interpolation comparisons

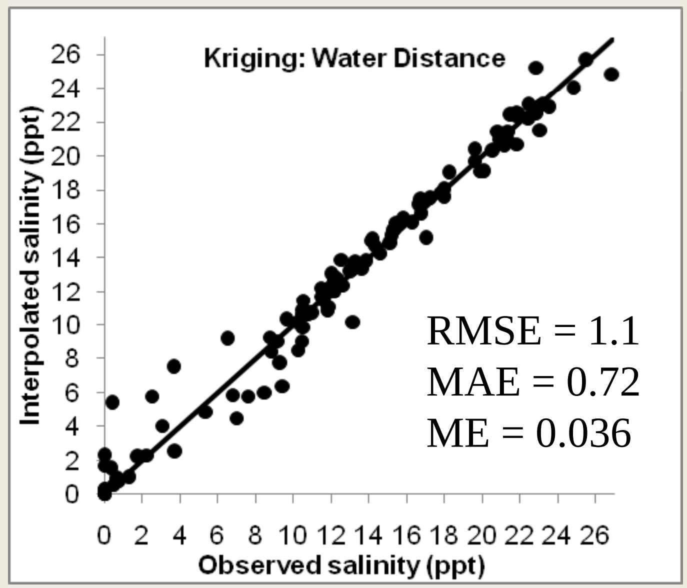
July 2007 Surface Salinity



Cross validation of surface interpolation results

- Hold out each sample, one at a time, and predict at the sample location
- Examine on plots, compute average errors



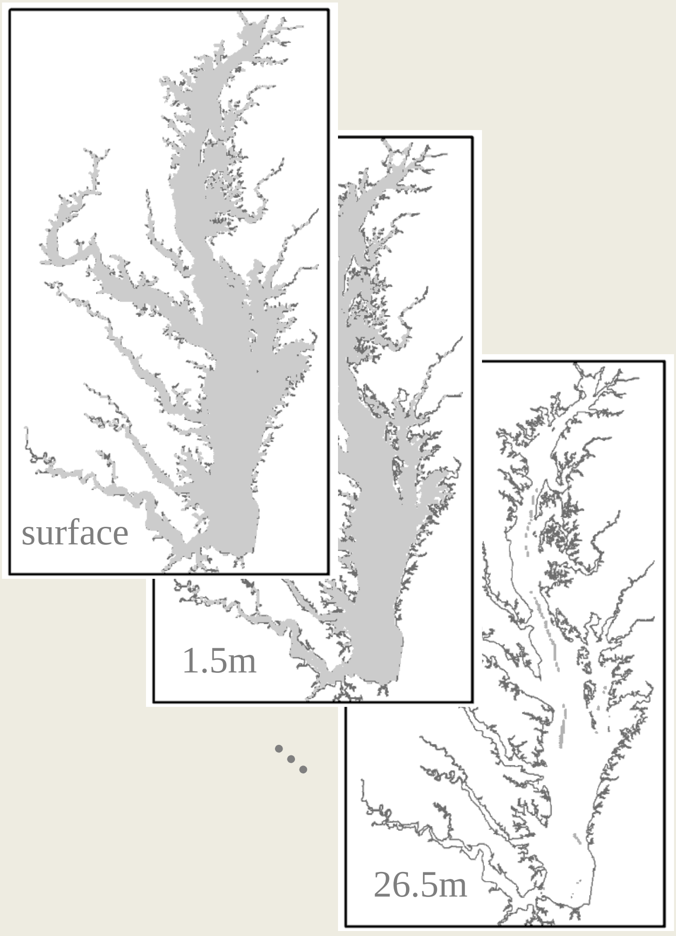


Water-distance-based method: Layers

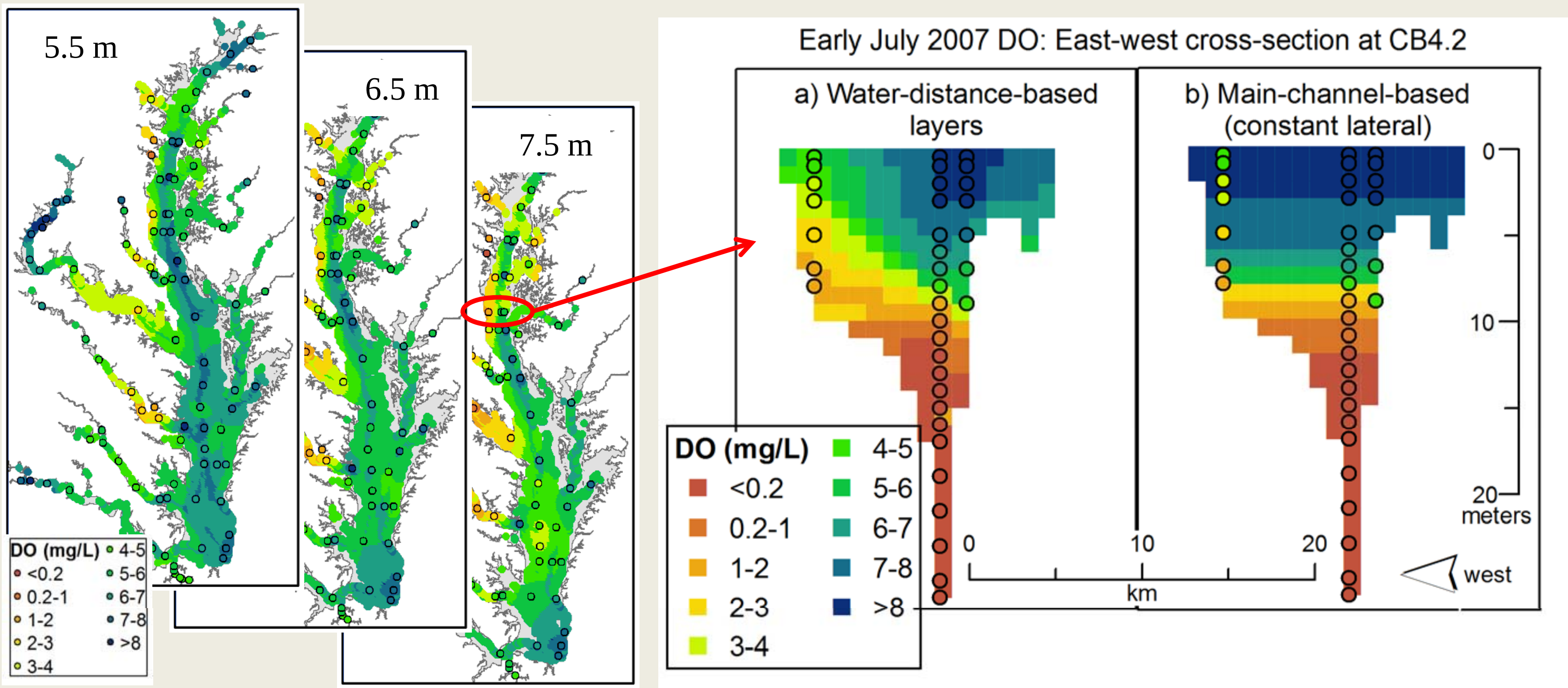
- Apply water-distance-based interpolation to data at every 1-m of depth
- To improve the vertical estimates -- use an indicator covariate as to whether each depth is above or below the pycnocline

$$DO(s) = \beta_0 + \beta_0 P(s) + \varepsilon(s)$$

P(s) = pycnocline indicator
β_i = fitted coefficient
ε(s) = spatially varying random error



Water-distance-based method: 3-D output



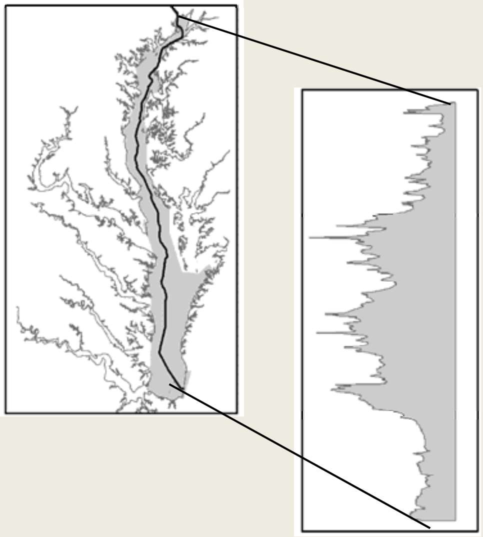
Overall: Water-distance-based method

- Good in shallow water
- Captures lateral mainstem patterns
- Some problems at deeper depths
- Can be used to compute hypoxic volume for the full bay

Outline

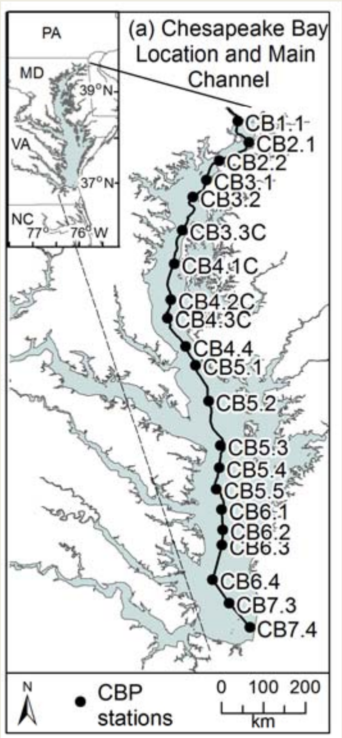
- What method(s) do you use for assessing DO?
- Why did you choose that methodology?
- What have you found drives DO patterns in the Bay?
  - Averaging period impacts perceived trend
  - Stratification and nitrogen loads
- What lessons have you learned that we should consider as we move forward?

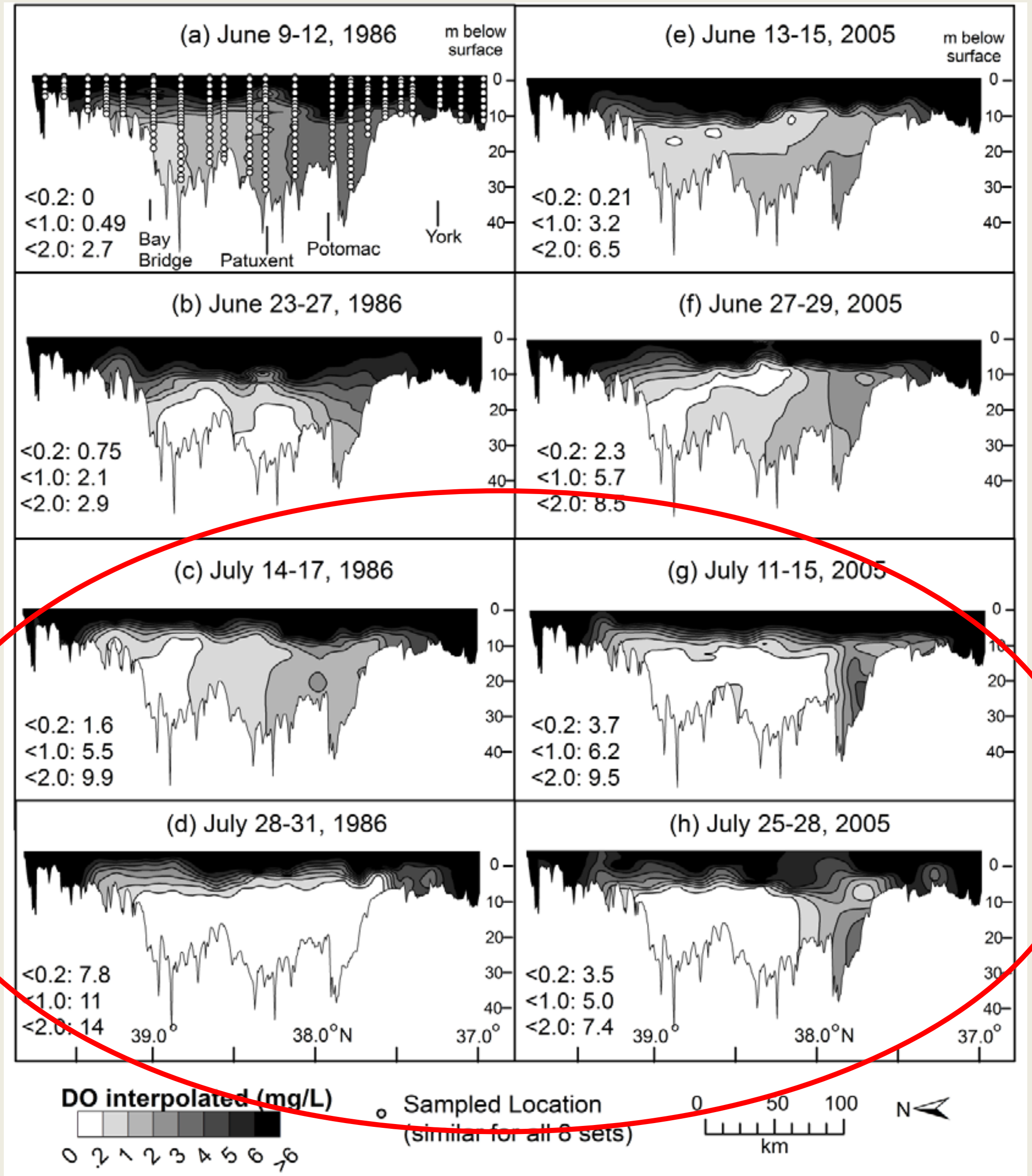
Main-stem method



Main channel DO examples:

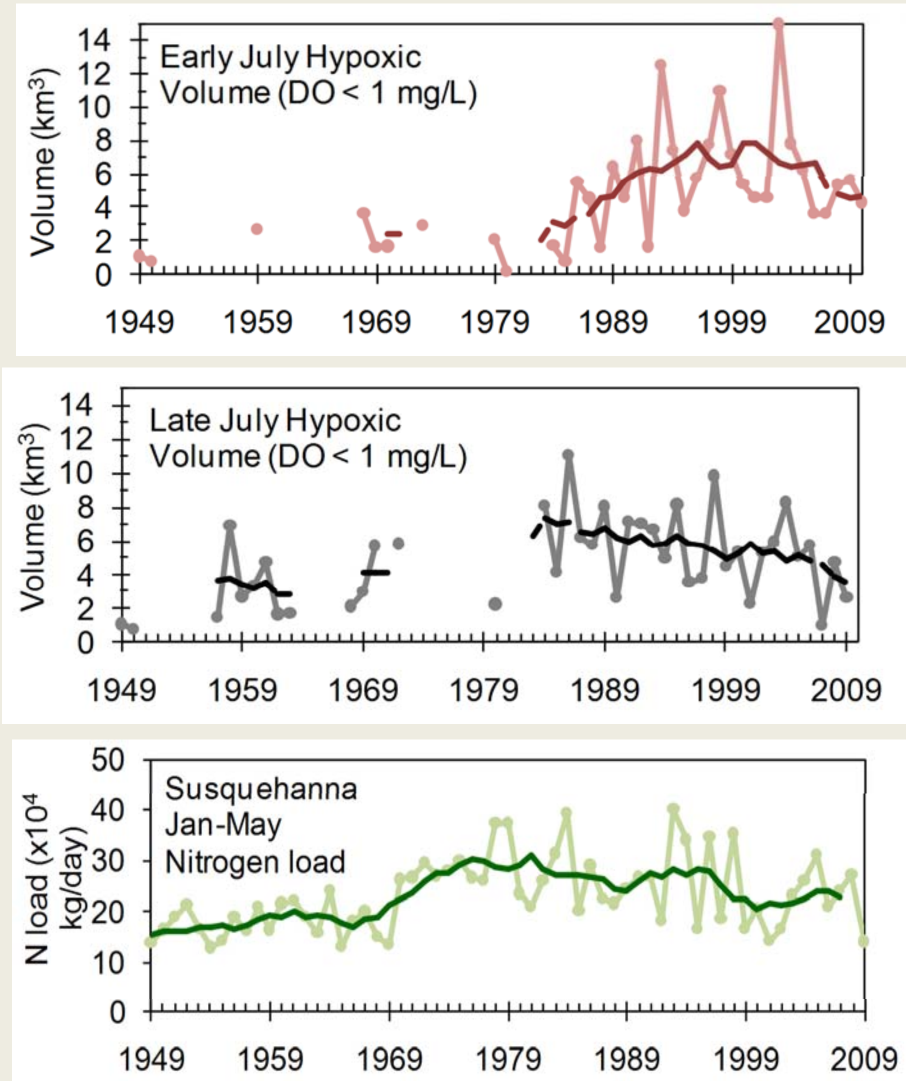
June and July 1986 and 2005





Murphy, Kemp, and Ball . 2011. *Estuaries and Coasts* 34:1293-1309.

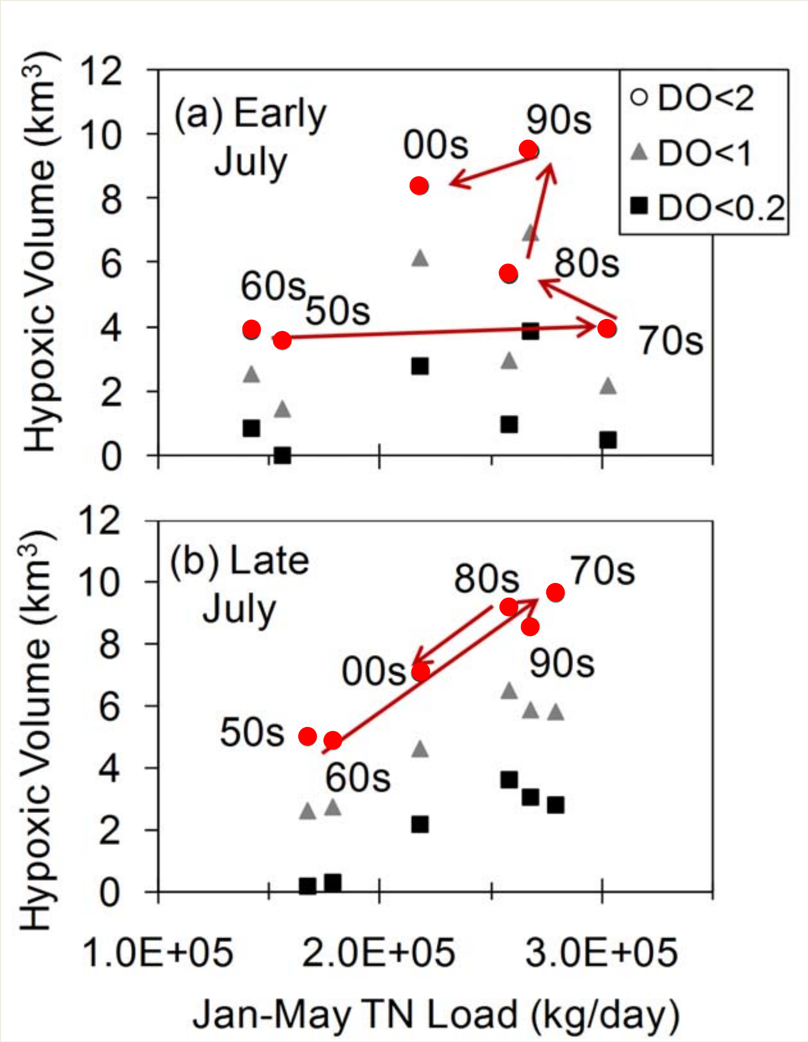
Hypoxia trends in relation to N-loading



- Early July hypoxia shows increase since 1980
- Inter-annual variations blur long-term trends; clarify with running means
- Late July hypoxia has actually declined since 1980s
- N-loading increased until mid-1980s, then declined gradually into 2000s
- Hypoxia and late July N-load significantly correlated ($p<0.001$)

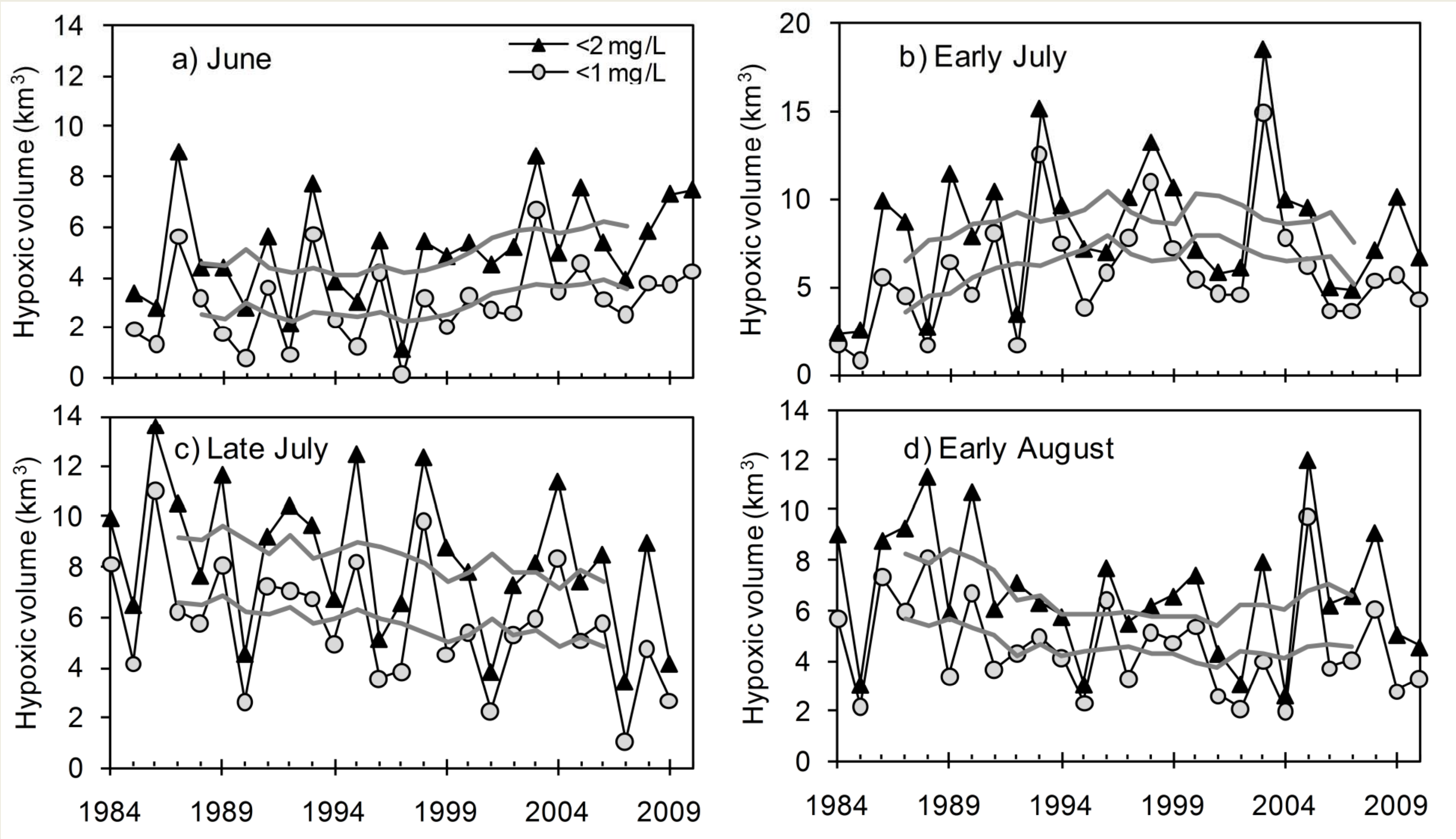
From: Murphy *et al*. 2011.

Decadal average hypoxic volume vs. TN



From: Murphy *et al*. 2011.

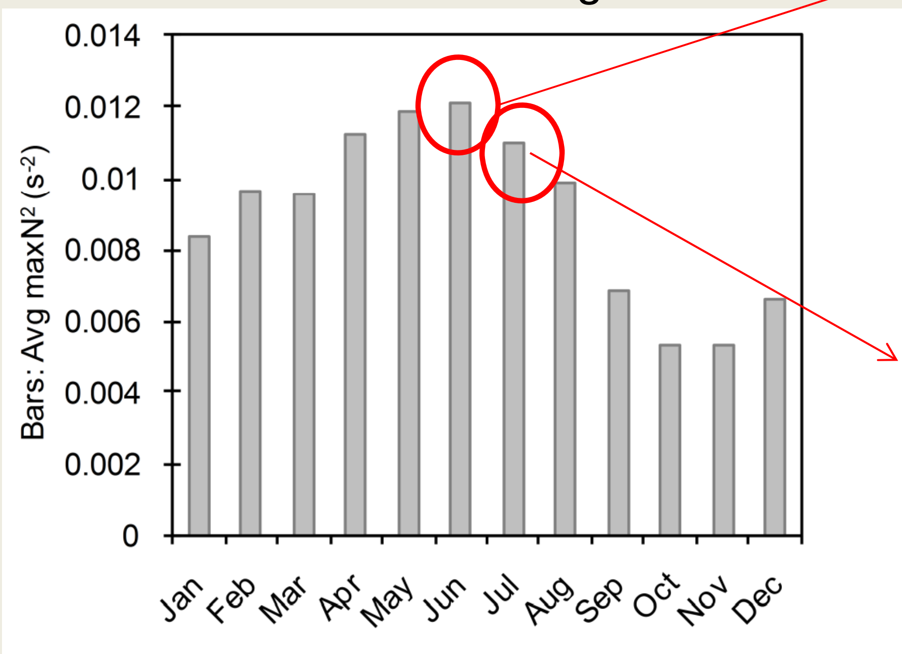
Entire summer hypoxic volume trends

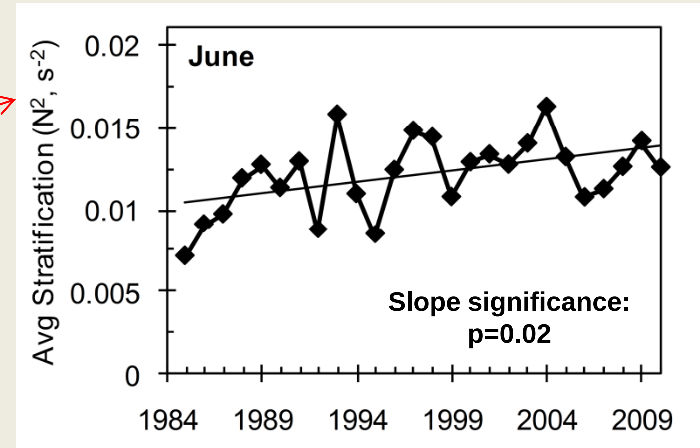


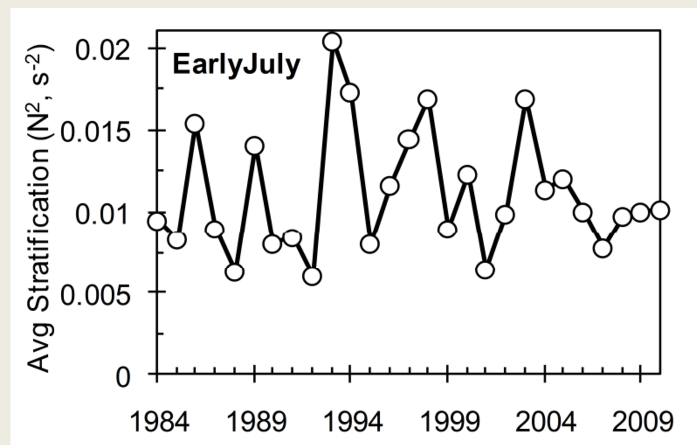
From: Murphy *et al*. 2011.

Stratification long-term patterns

Average Monthly Main Channel Stratification Strength



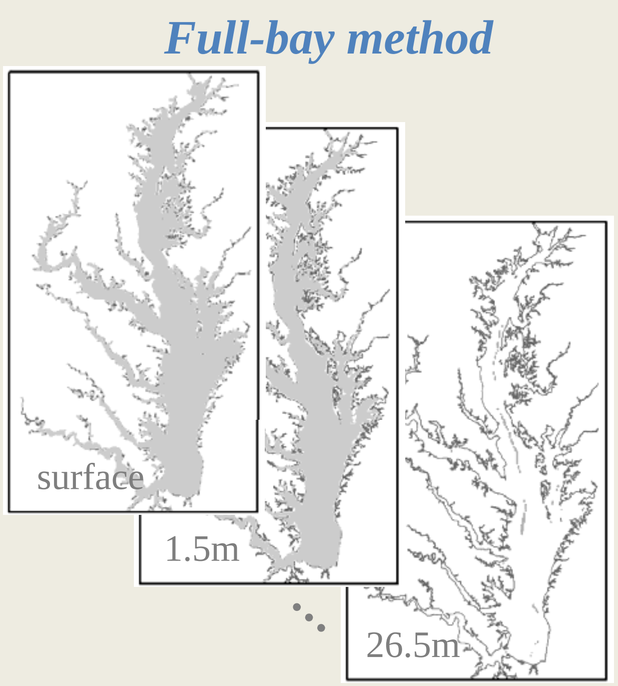




From: Murphy *et al*. 2011.

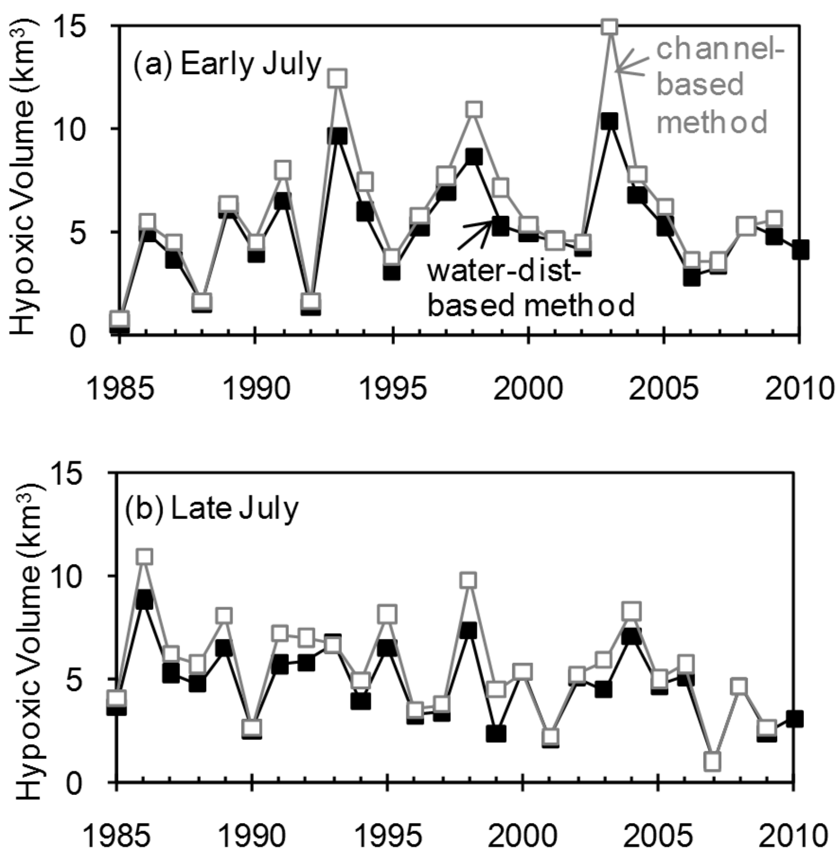
Outline

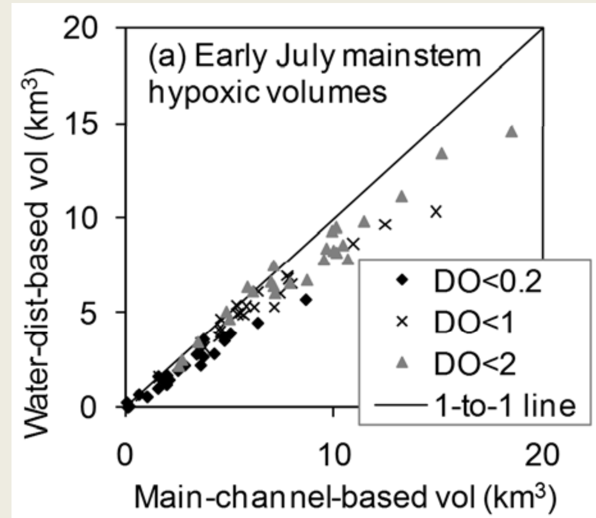
- What method(s) do you use for assessing DO?
- Why did you choose that methodology?
- What have you found drives DO patterns in the Bay?
  - Main channel hypoxia drives full-bay long-term trends
- What lessons have you learned that we should consider as we move forward?

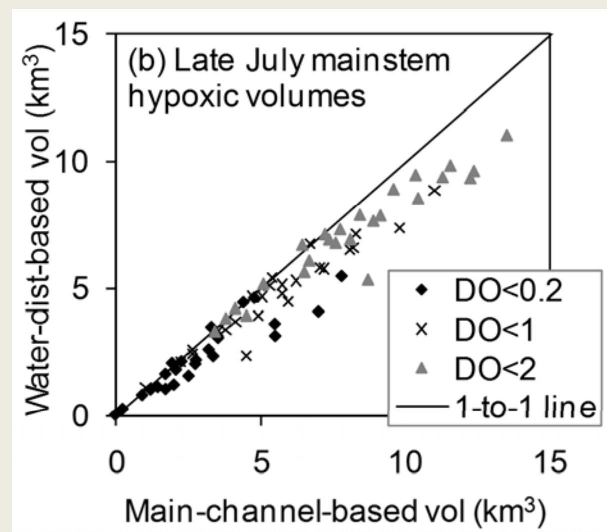


Re-evaluation of hypoxic volume trends

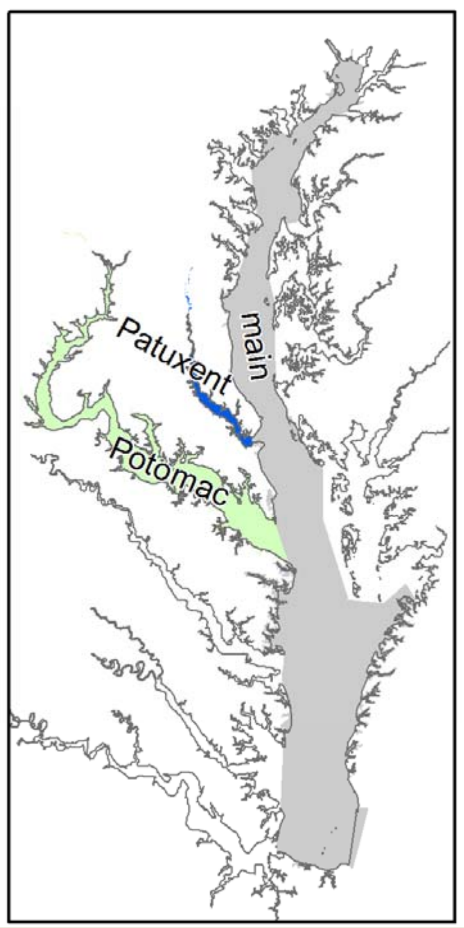
Mainstem Hypoxic Volume (DO<1 mg/L)

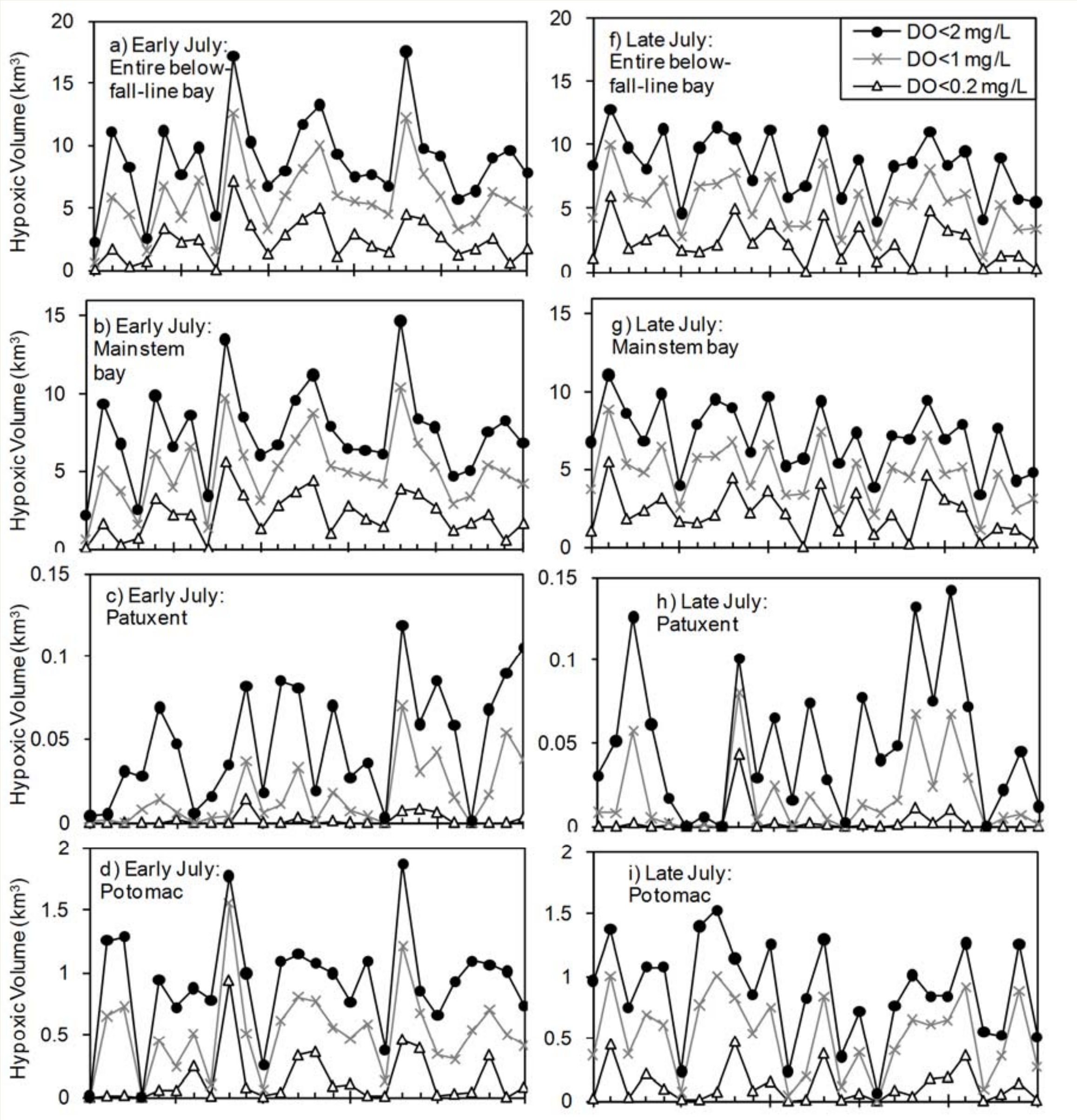






Results Part 2: Water distance





Conclusions

- What have you found drives DO patterns in the Bay?
  - A trend in early summer stratification appears to have lead to an increase in early summer hypoxic volume.
  - The different early and late summer hypoxic volume trends observed are not artifacts of the main-channel-only interpolations.
  - More specific analysis could be done in tributaries.

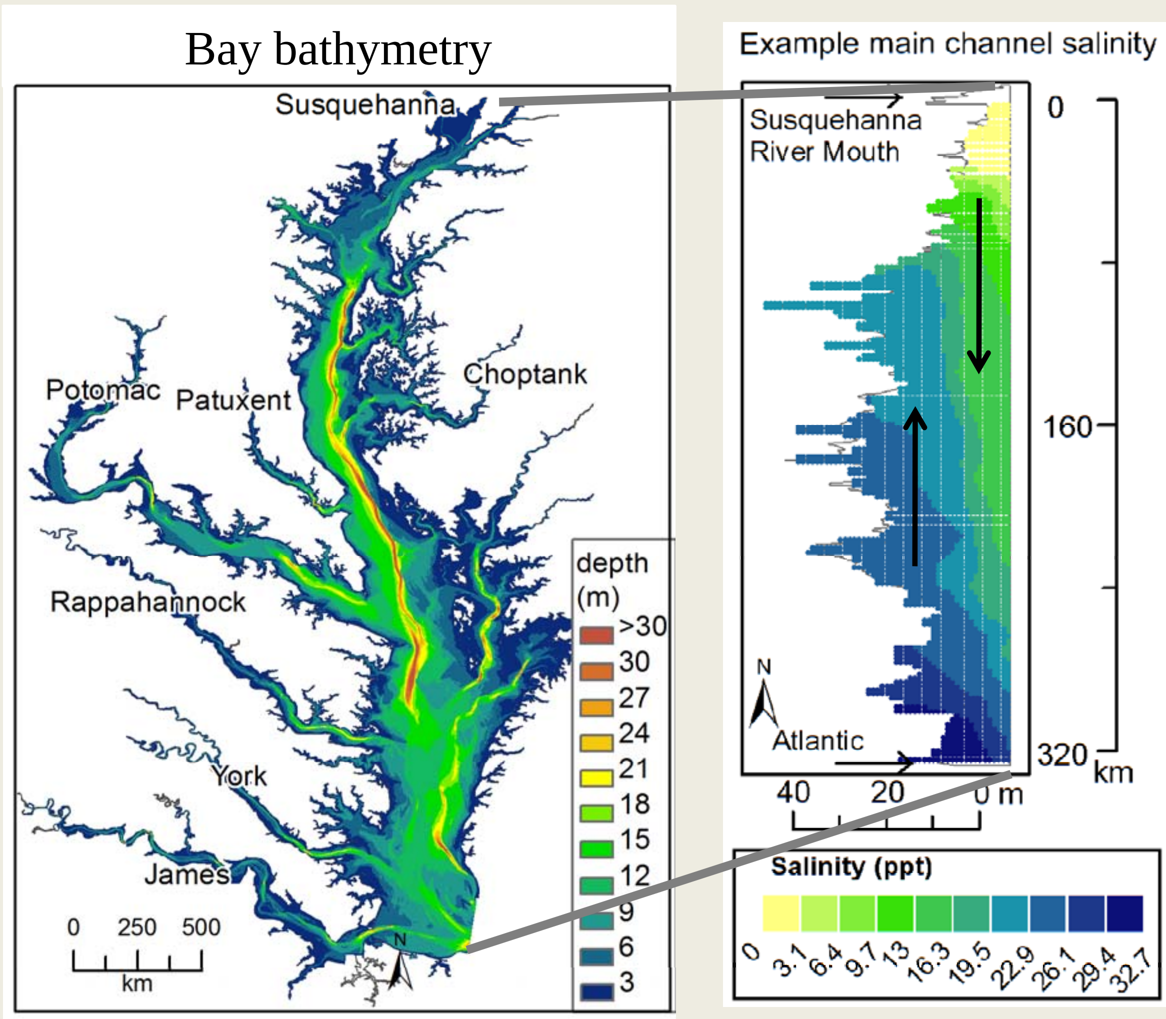
- What lessons have you learned that we should consider as we move forward?
  - Timing is important when analyzing hypoxia.
  - Average monthly or summer hypoxia estimates may result in lost information.

Acknowledgements

- JHU Advisor: Bill Ball
- Committee members: Grace Brush, Frank Curriero, Dominic Di Toro, Michael Kemp
- “Distance” sources: Eric Perlman and Andrew Miglino
- CBEO team: Randal Burns, Damian Brady, Jen Bosch, Jeremy Testa, Maureen Brooks
- Data sources: CBP, CBI, USGS, NOAA, MDNR, VECOS
- NSF Grants no. 0618986 and 0854329
- EA Science, Engineering, Technology

Extras

Chesapeake Bay

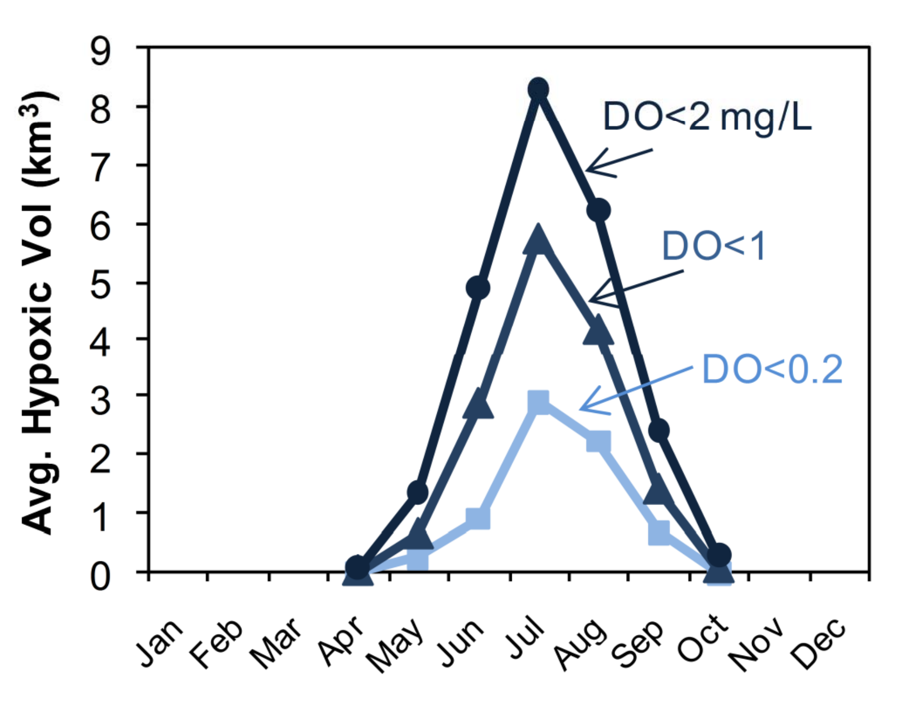


Bathymetry data from NOAA

- Bay is on average 6.5 m deep, but a much deeper channel follows the center of the Bay
- Most of the year, the Bay is stratified with fresher water on top, saltier water on bottom

Hypoxic volume: Temporal extent

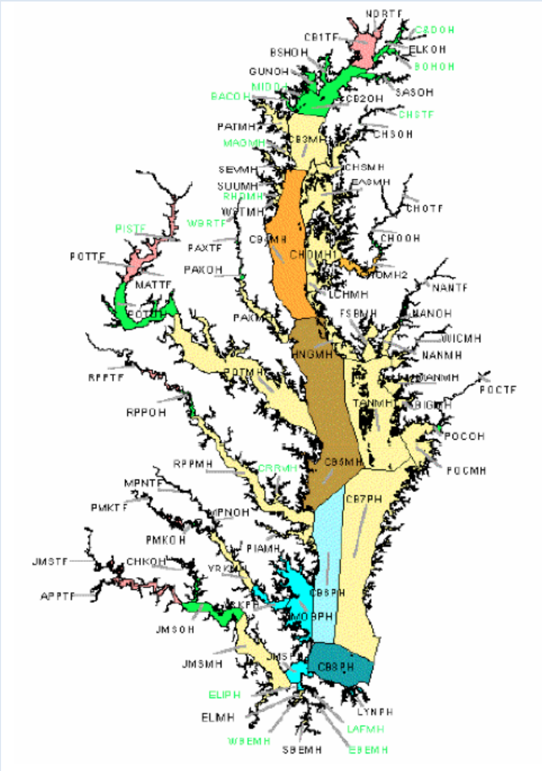
<u>Hypoxic volume</u> = volume of water with dissolved oxygen (DO) below certain critical values



Data summarized from: Murphy, Kemp, and Ball. 2011. *Estuaries and Coasts* 34:1293-1309.

Interpolation method used for management

1. Split bay into segments and 1-m depth layers

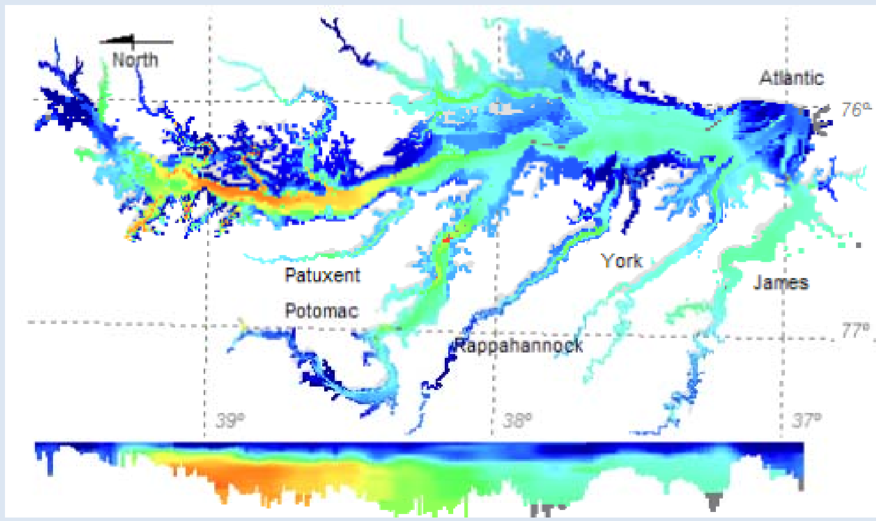


Chesapeake Bay Program 1998 segmentation design.

2. Interpolate samples in or near each segment using IDW

$$\hat{Y}(s_0) = \sum_{i=1}^{n} w(s_i) Y(s_i) \qquad w(s_i) = \frac{1/d_i^2}{\sum_{j=1}^{n} \left(1/d_j^2\right)}$$

4. Combine interpolation output by segment and layer



Images from Vol36 User's Guide (Bahner 2006)

Variogram

Classical Variogram Estimator

$$2\hat{\gamma}(\mathbf{h}) = \frac{1}{|N(\mathbf{h})|} \sum_{N(\mathbf{h})} (y(\mathbf{s}_i) - y(\mathbf{s}_j))^2$$

- $N(\mathbf{h})$ contain the pairs of locations $(\mathbf{s}_i, \mathbf{s}_j)$ that are a distance $\|\mathbf{h}\|$ apart, $\mathbf{h} = \mathbf{s}_i - \mathbf{s}_j$.
- $|N(\mathbf{h})|$ is the number of such pairs.

From Frank Curriero

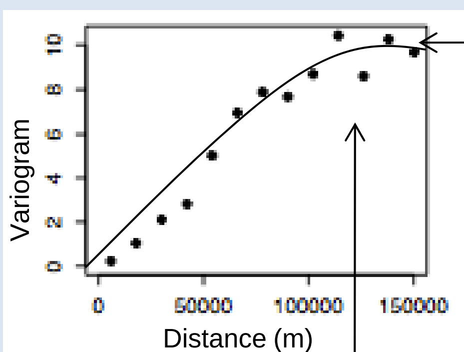
Some notes on kriging

Variogram

1. Examine an empirical variogram of observed data $\mathbf{Y_2}$ as a function of the Euclidean distance between points

$$2\hat{\gamma}(h) = \frac{1}{|N(h)|} \sum_{N(h)} \left[Y(s_i) - Y(s_j) \right]^2$$

$s_{i,j}$ are locations
N(h) is number of pairs distance h apart



sill

range

2. Fit a valid variogram model

Estimate unknown values $\mathbf{Y_1}$ given $\mathbf{Y_2}$

3. Use variogram model to fill in covariance matrix:

$$\mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{bmatrix}$$

4. Use the conditional distribution of the unobserved data given the observed to generate estimates for Y_1

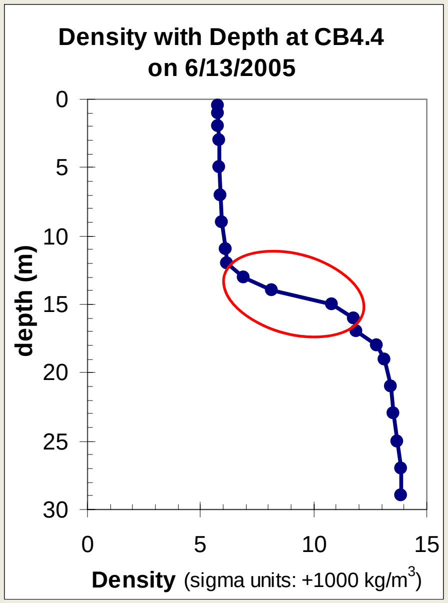
$$E(\mathbf{Y}_1 \mid \mathbf{Y}_2) = \mu_1 + \mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}^{-1}(\mathbf{Y}_2 - \mu_2)$$

μ_2 is mean of observed data, μ_1 is mean of unknown values (predicted using stationarity assumption)

Optional: Include covariates to account for some spatial variability in μ (universal kriging)

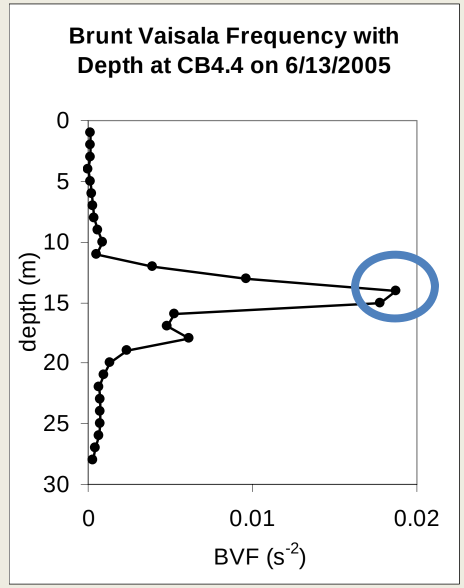
Hypoxia/Stratification

Calculation of stratification strength

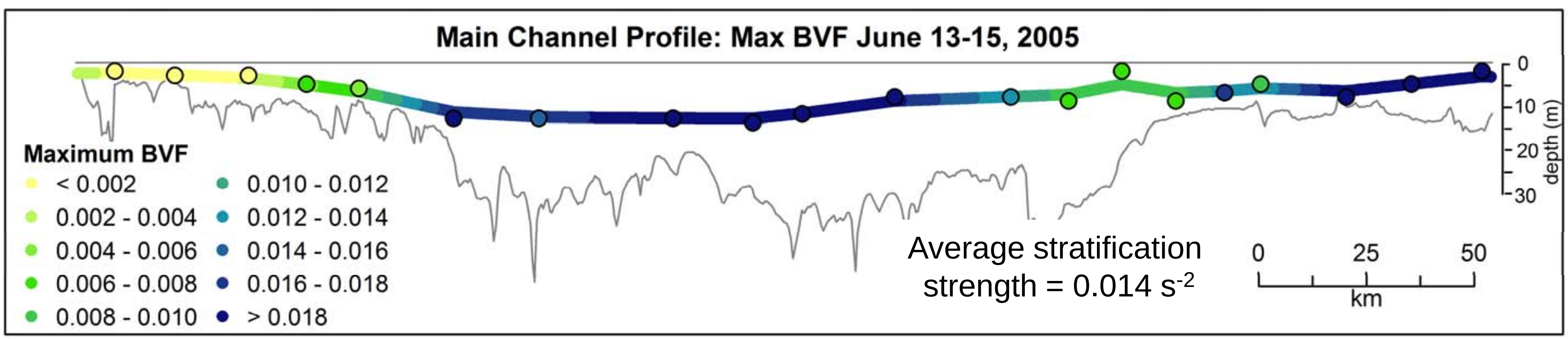


1. Calculate Brunt Väisälä Frequency

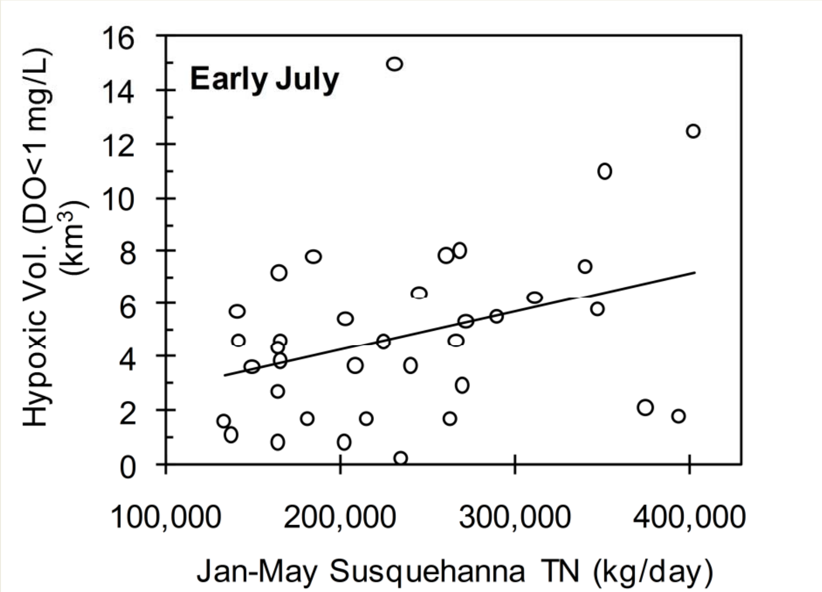
$$BVF = \frac{g}{\rho}\frac{\partial \rho}{\partial z}$$

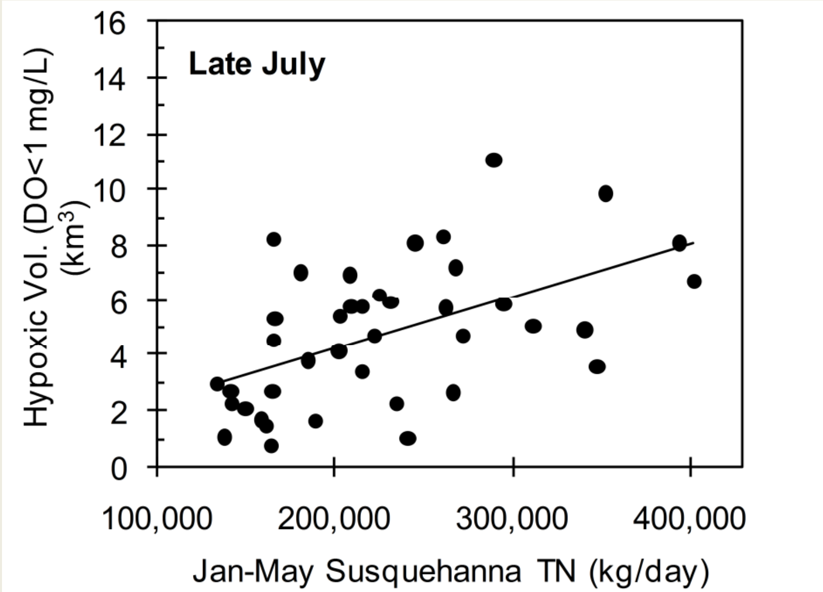


2. Interpolate maximum Brunt Väisälä Frequency (BVF)



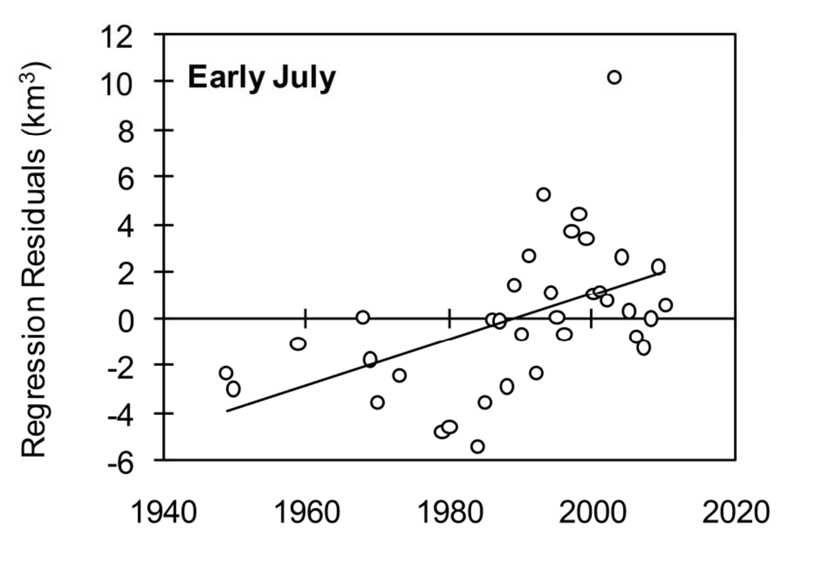
Hypoxic volume vs. TN

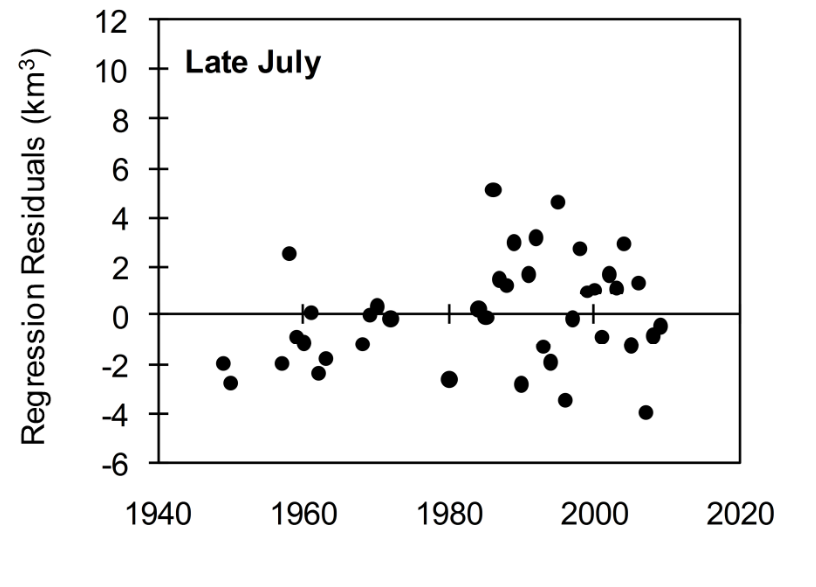




Regression Model	HypoxicVol=β_0+β_1(TN)
Early July (DO<1 mg/L)	R^2=0.12, p-value=0.04
Late July (DO<1 mg/L)	R^2=0.28, p-value<0.001

Hypoxic volume vs. TN residuals

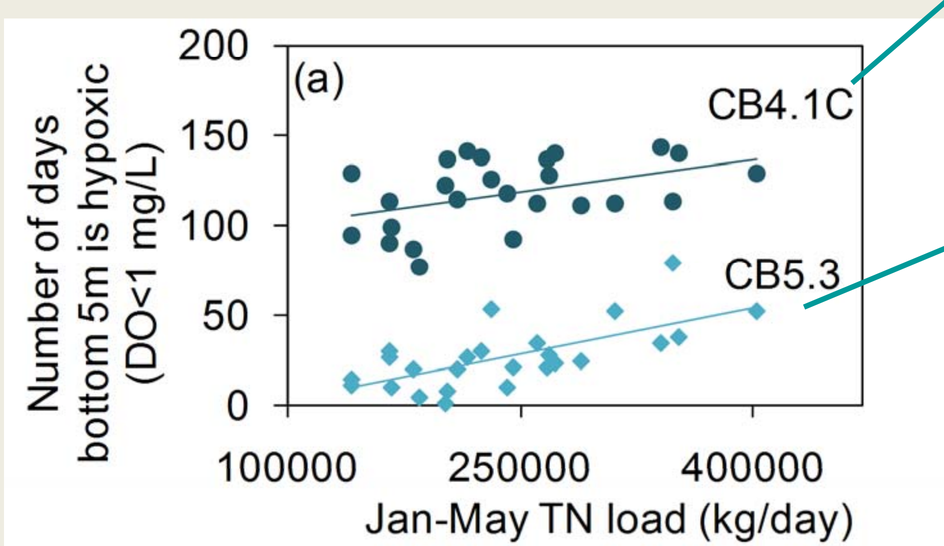


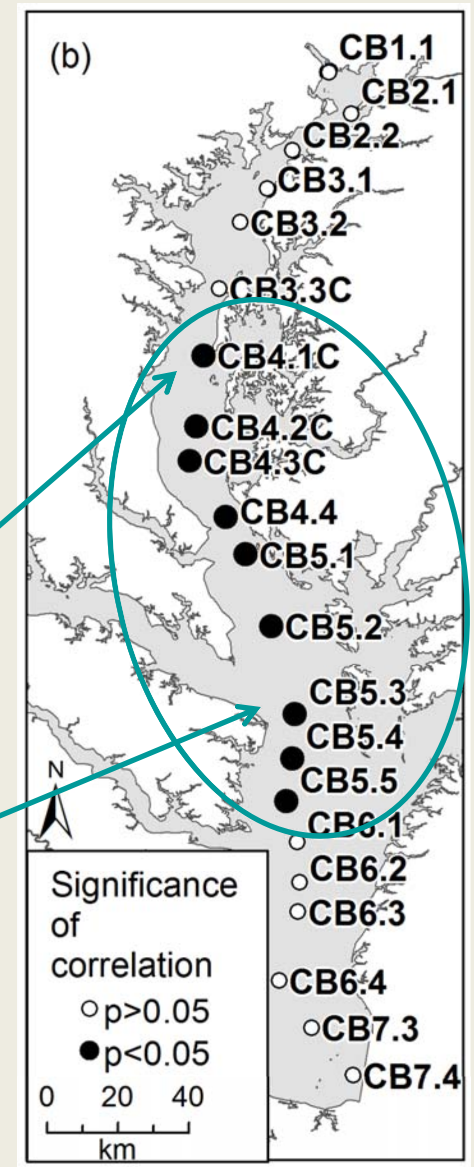


Regression Model	HypoxicVol=$\beta_0+\beta_1$(TN)	Residuals=$\beta_0+\beta_1$(year)
Early July (DO<1 mg/L)	R^2=0.12, p-value=0.04	R^2=0.25, p-value=0.001
Late July (DO<1 mg/L)	R^2=0.28, p-value<0.001	R^2=0.07, p-value=0.1

Hypoxia Duration

- Number of days that bottom 5 m of water are hypoxic
- In mid-Bay, the hypoxia duration is significantly correlated with Jan-May TN loads





From: Murphy *et al*. 2011.

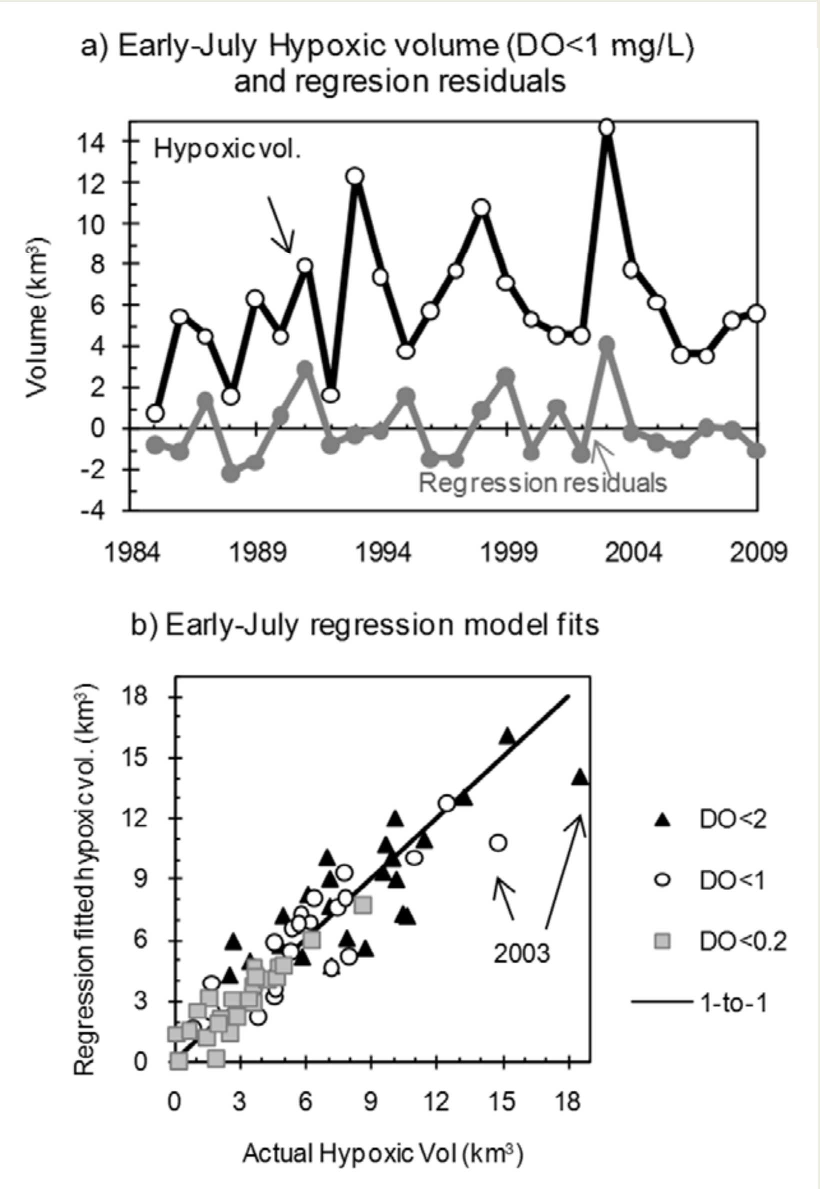
Regression for hypoxic volume (DO<1 mg/L)

$$HypoxicVol_{EarlyJuly} = \beta_0 + 1.2\,(Stratification_{June}) + 1.8\,(Stratification_{EarlyJuly}) + 0.5\,(VolBelowPyc_{EarlyJuly}) + \varepsilon$$

$R^2=0.77$, $p<0.001$

June stratification is only variable that explains the temporal increase

From 1985-2009

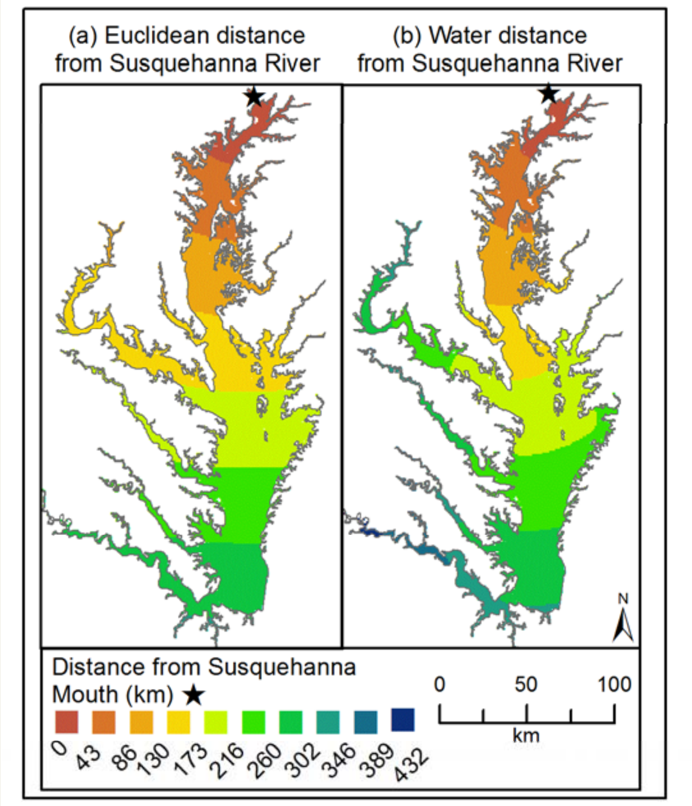


From: Murphy *et al.* 2011.

Water distance

Water distance

- Distance between locations through water
- Computed between 11,534 grid and sample locations



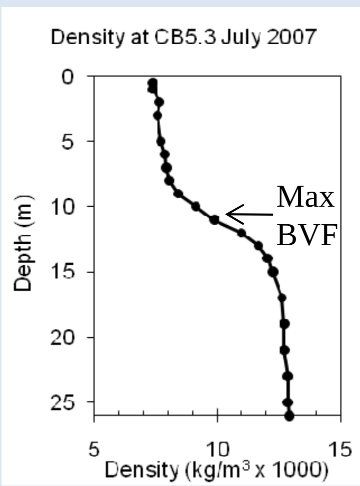
Water distances computed by Eric Perlman (was at JHU CS)

Method 2: Full Bay

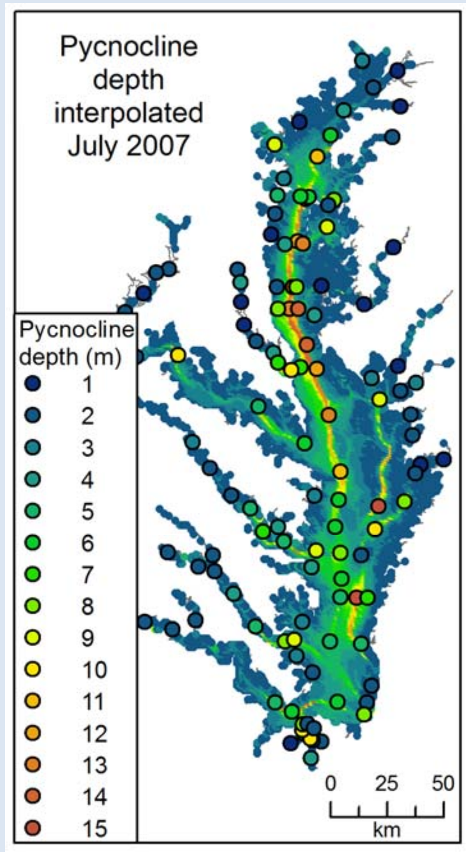
Water-distance-based method: Layers

1. Identify depth of pycnocline

$$BVF = \frac{g}{\rho}\frac{\partial \rho}{\partial z}$$



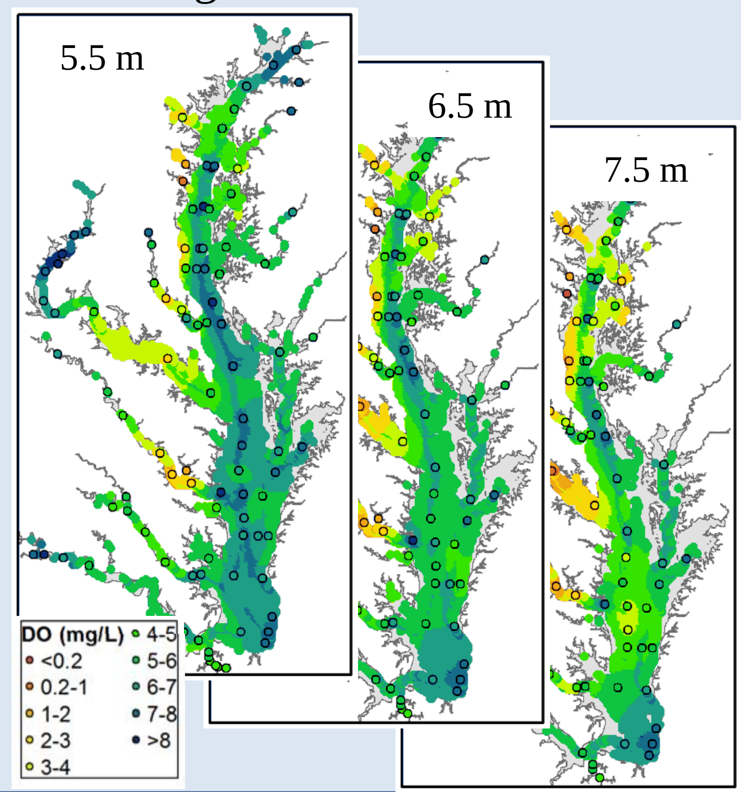
2. Interpolate throughout bay



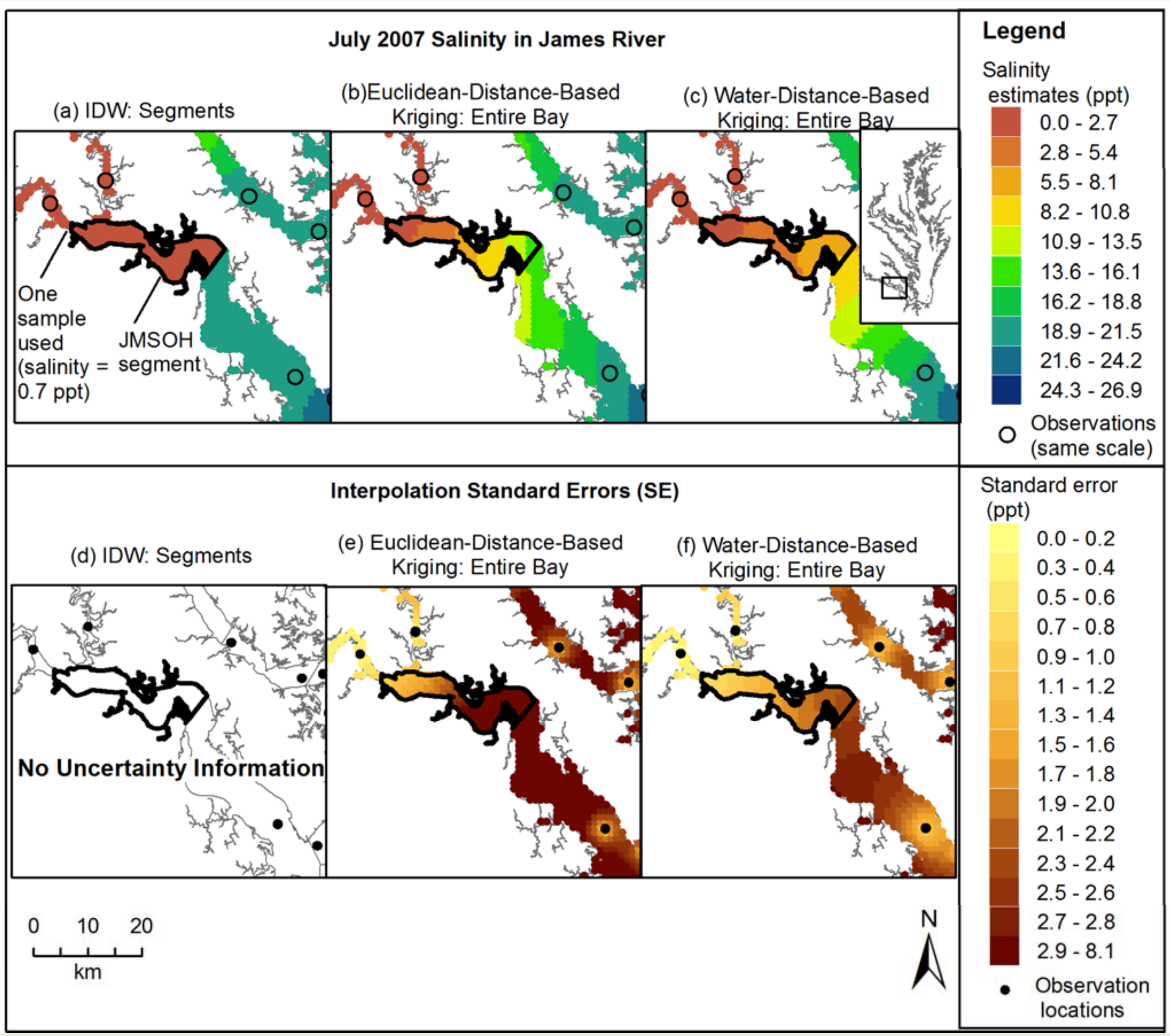
3. Use pycnocline depth indicator (P) as a covariate to interpolate DO at location s

$$DO(s) = \beta_0 + \beta_0 P(s) + \varepsilon(s)$$

4. "Stack" interpolated DO layers to generate 3-D estimate



Interpolation Results



Cross Validation Summary

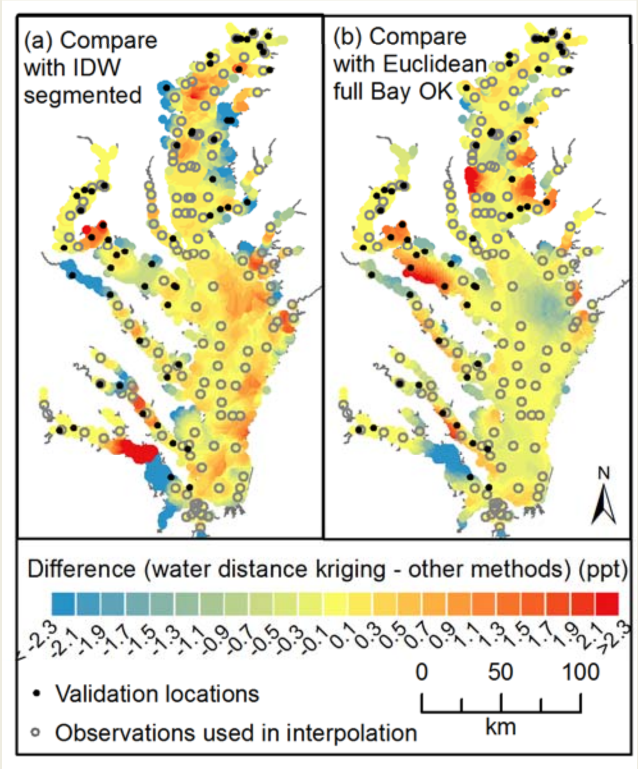
RMSE for July 2007 (and percent of time method has lowest RMSE for all 2007/2008 sets)

Parameter	IDW in segments	Kriging with Euclidean distance	Kriging with water distance
Water temp	0.79 (12%)	0.76 (8%)	**0.74 (80%)**
Salinity	2.3 (0%)	1.5 (0%)	**1.1 (100%)**
DO	1.5 (0%)	**1.2** (8%)	**1.2 (92%)**
NH_4	0.023 (16%)	**0.022** (20%)	0.023 **(64%)**
$NO_2 + NO_3$	0.18 (12%)	0.25 (16%)	**0.17 (72%)**
PO_4	0.0079 (4%)	**0.0073** (12%)	0.0075 **(84%)**
Chl-a	**15** (8%)	**15** (32%)	**15 (60%)**

Validation Test

- Identify continuous monitoring stations from Maryland Department of Natural Resources and Virginia Estuarine and Coastal Observing System
- Average continuous observations 1 hour before and after the time of closest CBP sample
- Compare validation observation to interpolation output

Surface Salinity July 2007: Difference between water distance kriging and other methods and validation locations



Validation: http://www3.vims.edu/vecos/
http://mddnr.chesapeakebay.net/newmontech/contmon/index.cfm

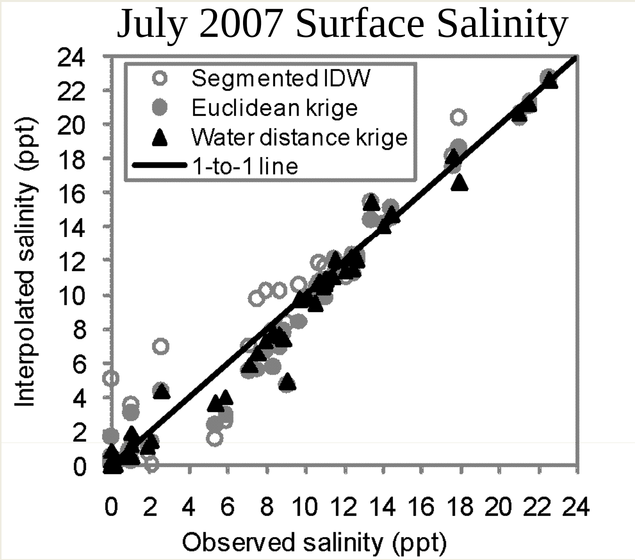
Validation Results

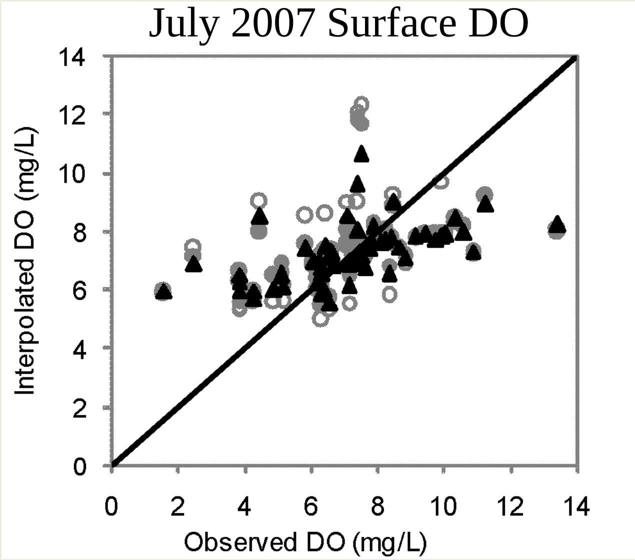
Root Mean Squared Errors of Estimates

	IDW in segments	Kriging with Euclidean distance	Kriging with water distance
Water temp	1.0	0.88	**0.84***
Salinity	1.4	1.2	**0.92**
DO	2.0	1.9	**1.8**
Chl-a	29	24	**21**

*Uses a covariate, depth

Validation sets: Maryland Department of Natural Resources and Virginia Estuarine and Coastal Observing System continuous monitoring data





Hypoxic volumes computed using water-distance-based method