Fusing Surface Monitors, Satellites and Forecasts for Near-real-time Air Quality

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22nd Annual CMAS Conference - 2023-10-18

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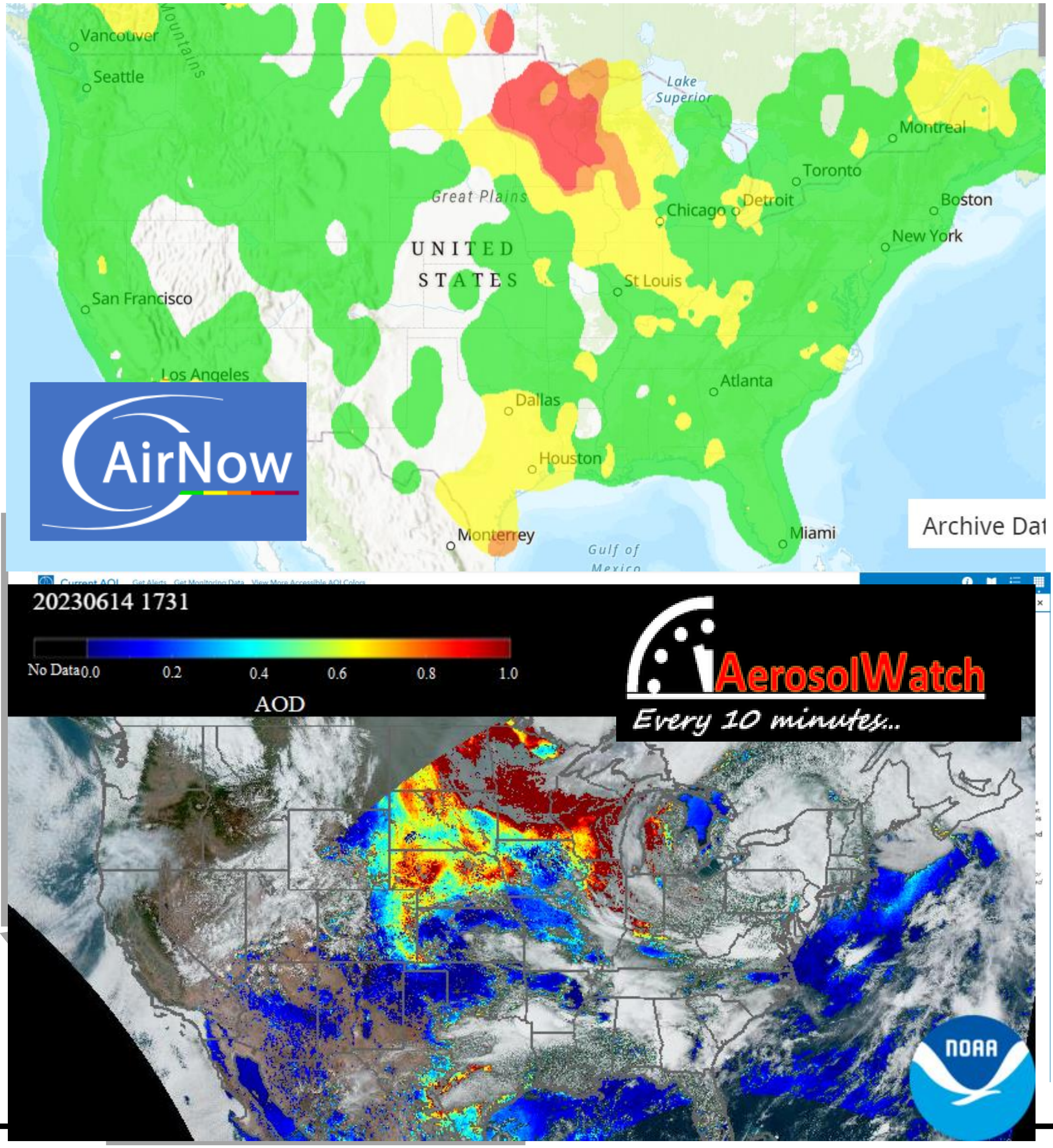
Motivation

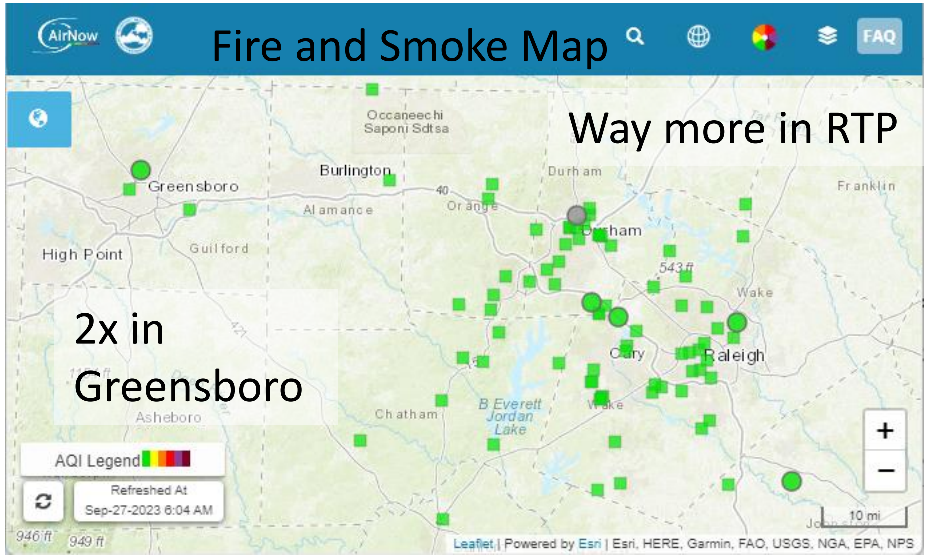
- AirNow communicates air quality in real time
  - Millions of visitors per day during fire seasons
  - Simple distance (d^{-5}) contours monitors only
- 4x more PurpleAir sensors than monitors
  - Increased the spatial coverage of monitored particulate matter.
  - Spoiler alert: sensor data improves predictions.
- Near-real-time satellite observations
  - Recent development by NOAA/NESDIS/STAR
  - NASA HAQAST project connecting AirNow to NOAA geostationary satellite data
- What about fusing AirNow, PurpleAir and satellites?

Example Day in AirNow and Aerosol Watch



Monitors and PurpleAir sensors

- Many agencies report monitor data to AirNow
  - ~1000 reporting monitors per hour
  - Publicly available thru AirNowAPI
- Schulte et al (2020) using PurpleAir
  - Residual Kriging with both AirNow and PurpleAir
    - NOAA Forecast model
    - Model Correction : $Y = M_n - \text{Krig}(M_n - O_n)$
  - Improved performance of PM2.5 in leave-one-out validation and compared to Federal Reference Monitors
- We use corrected PurpleAir low-cost sensors
  - Barkjohn et al. 2021 developed a national correction
  - Extended correction via RSIG



Better RMSE in Los Angeles

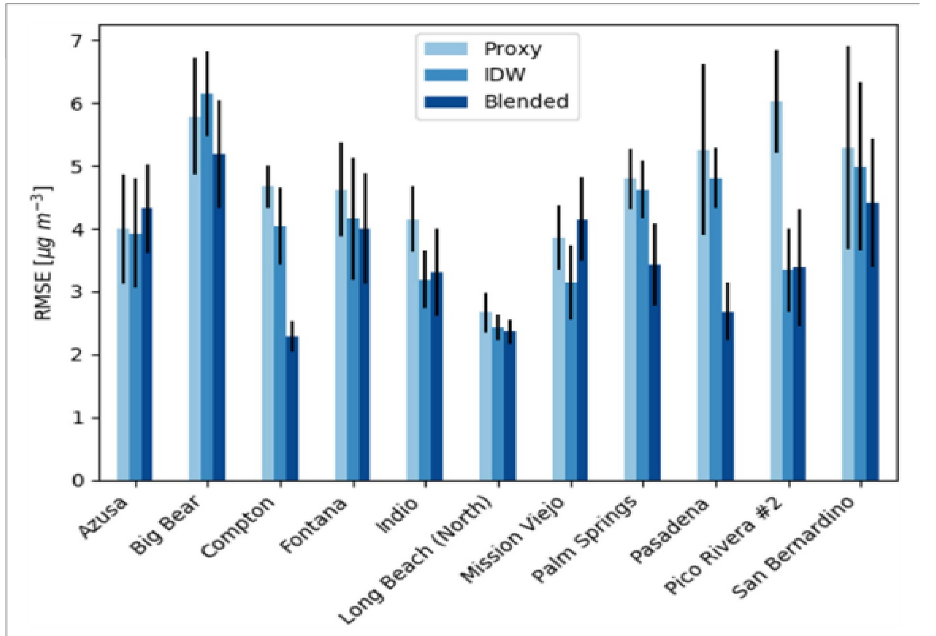


Figure 2. Root mean square error for $PM_{2.5}$ at each regulatory ambient monitoring station calculated using the independent gravimetric data. The RMSE is calculated from the 24-hour average concentrations. Vertical black solid lines are 95% confidence intervals.

Schulte et al 2020 (10.1088/1748-9326/abb62b)

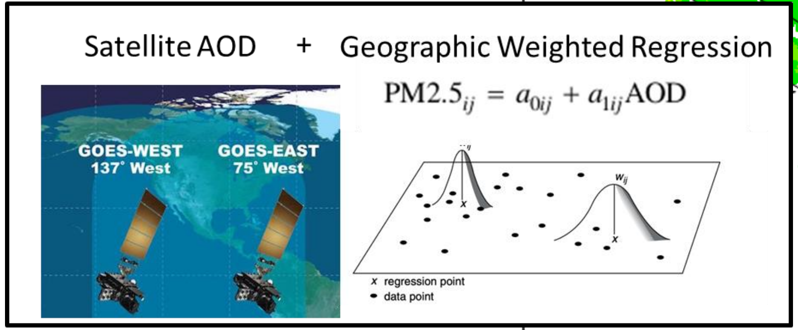
4. Enabling USEPA to ingest high-frequency satellite air quality data into the AirNow system

Team Lead: HAQAST investigator Pawan Gupta

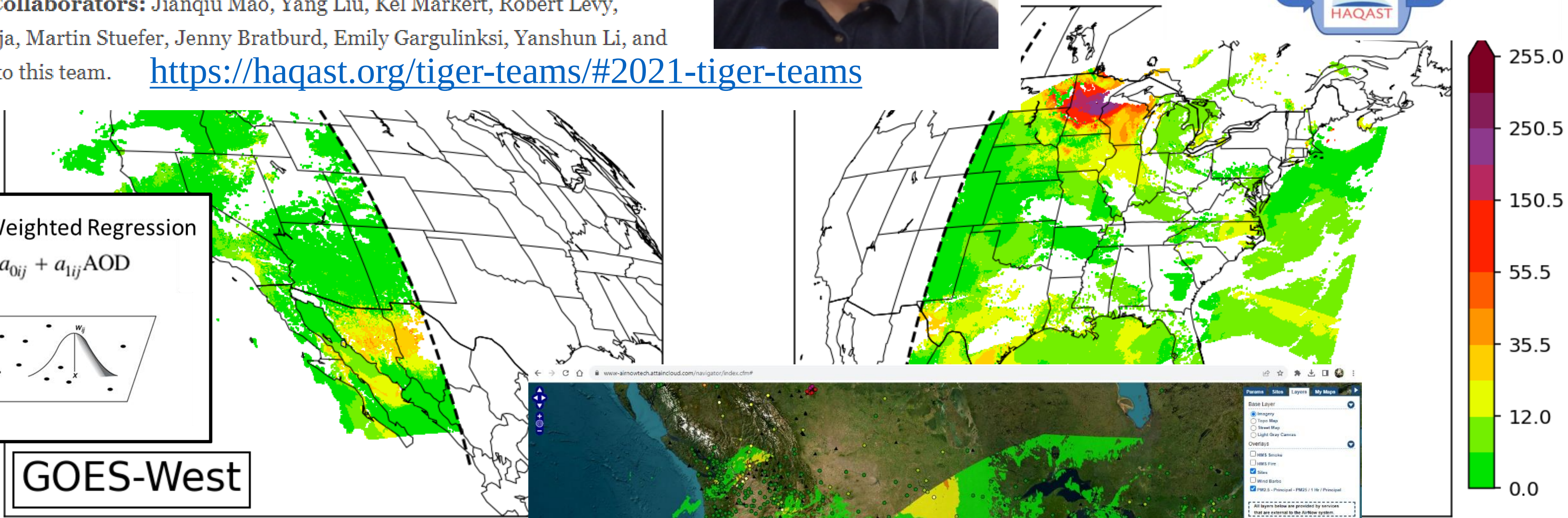
Partners: Phil Dickerson and Barron Henderson with the US Environmental Protection Agency (EPA), and Shobha Kondragunta with the National Oceanic and Atmospheric Administration (NOAA)

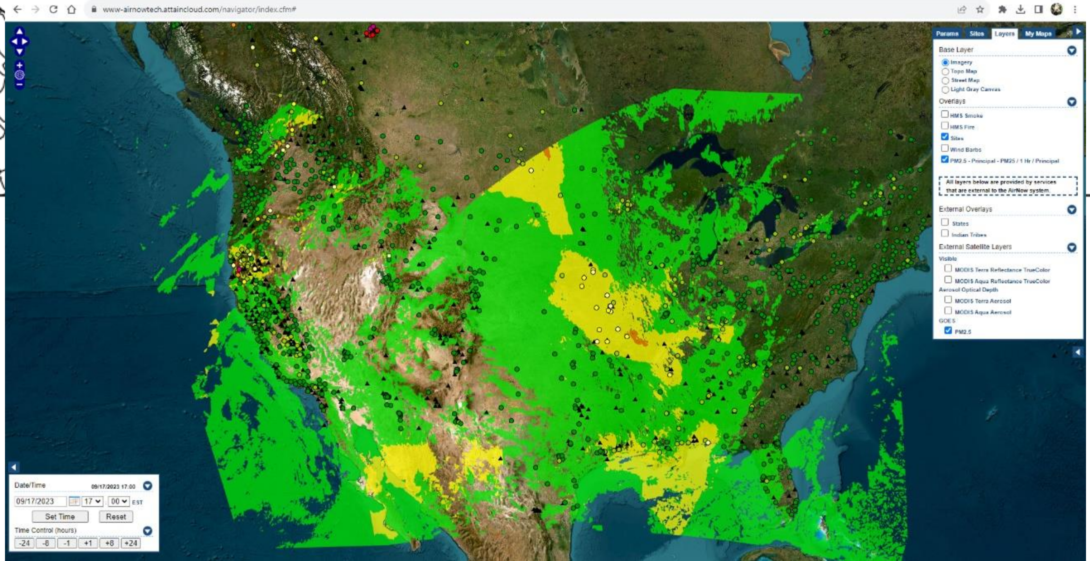
HAQAST Members and Collaborators: Jianqiu Mao, Yang Liu, Kel Markert, Robert Levy, Randall Martin, Amber J. Soja, Martin Stuefer, Jenny Bratburd, Emily Gargulinksi, Yanshun Li, and Daniel Tong also contribute to this team.

https://haqast.org/tiger-teams/#2021-tiger-teams



$$PM2.5_{ij} = a_{0ij} + a_{1ij}AOD$$





1.Sayeed et al: Deep Neural Network bias corrections.
2.O'Dell et al.: Public Health Benefits from Improved Identification of Severe Air Pollution Events with Geostationary Satellite Data, *submitted to GeoHealth*, 2023.
3.Zhang et al.: Nowcasting Applications of Geostationary Satellite Hourly Surface PM2.5 Data. Weather and Forecasting, 37(12), 2313-2329, 2022. doi: 10.1175/WAF-D-22-0114.1
4.Bratburd et al.: Air Quality Data When You Need It: Incorporating Satellite Data Updates into AirNow, EM Plus, 2022.
5.Zhang and Kondragunta.: Daily and Hourly Surface PM2.5 Estimation From Satellite AOD, Earth Space Sci, 8, doi: 10.1029/2020EA001599, 2021.

Hourly National-scale Fusion Ensemble

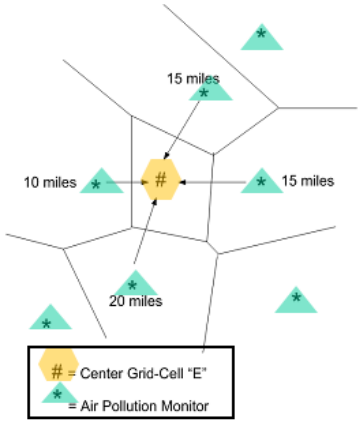
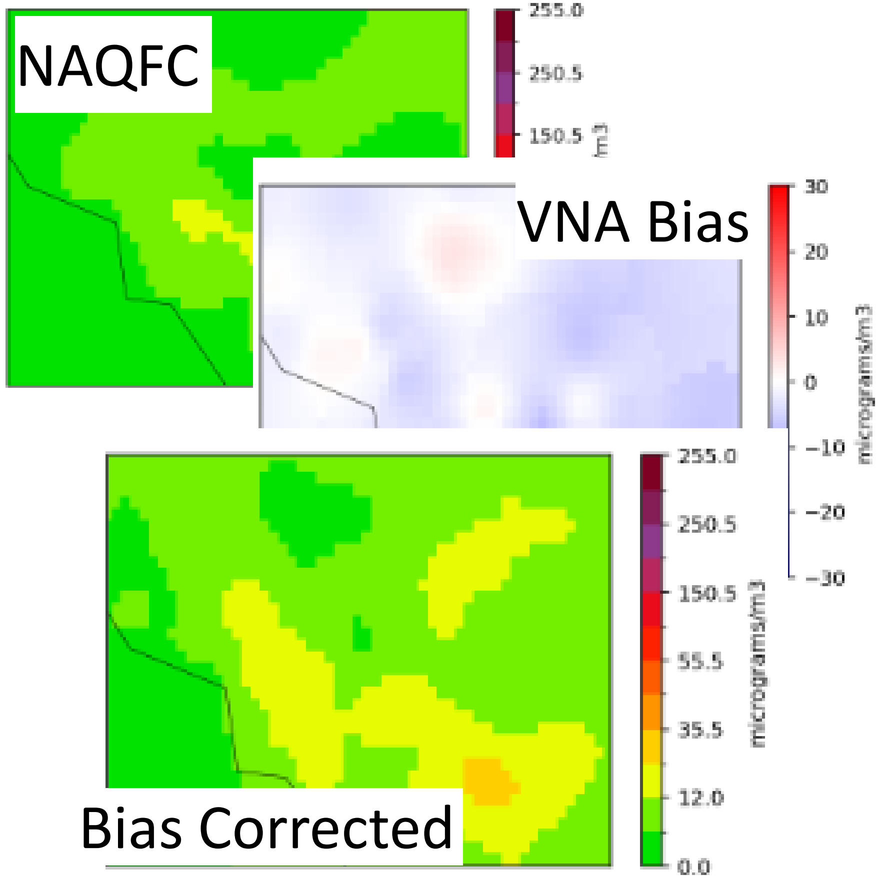


Figure courtesy of: Brian Timin

- Interpolating bias to "correct" the forecast model*
  - NOAA's Forecast Model (NAQFC) as mediating layer
  - VNA Bias = $\text{sum}(d_n^{-2}(m_n - o_n)) / \text{sum}(d_n^{-2})$
    - n = Voronoi Neighbor
  - Y_i = NAQFC – VNA Bias_i
- One layer from AirNow (Y_{AN}) ***observations***:
  - mostly regulatory grade hourly observations
  - paired with collocated grid cell.



*A multiplicative corrector of this type is called extended VNA (eVNA)
**Piece-wise regression as in Fire and Smoke Map

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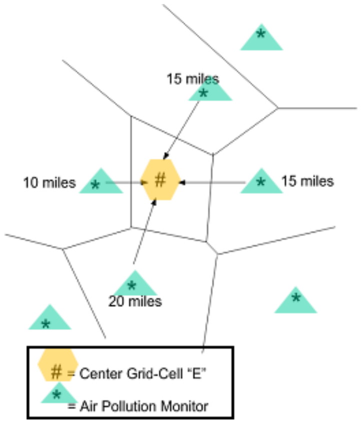

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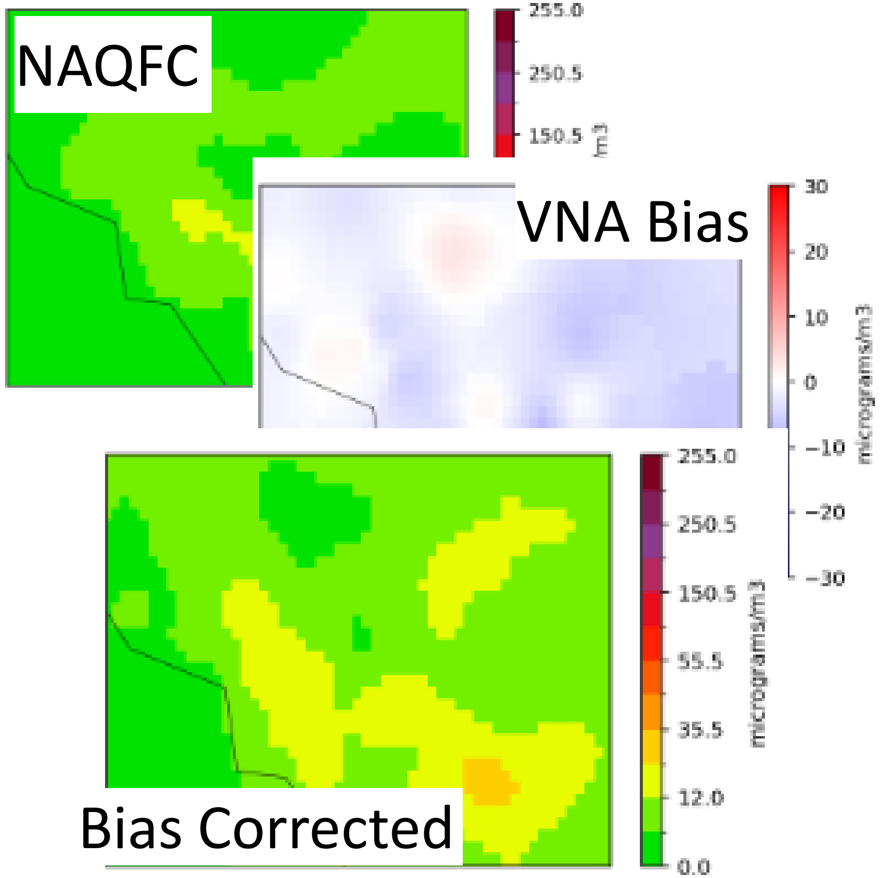
  - low-cost sensor hourly observations with calibration**
  - Aggregated within grid cells to create a pseudo-observation



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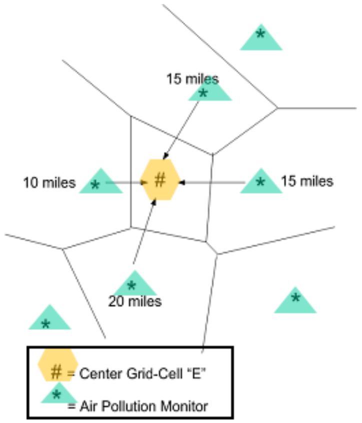

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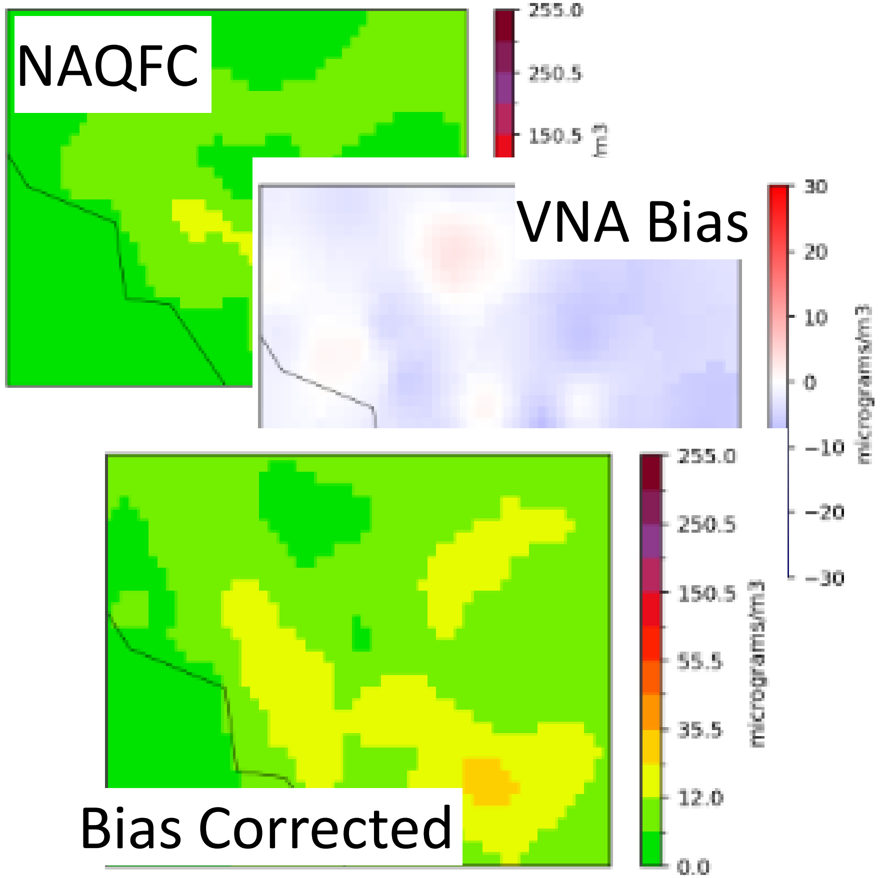
  - low-cost sensor hourly observations with calibration**
  - Aggregated within grid cells to create a pseudo-observation
- One layer from GOES-PM25 (Y_{GOES}) "***observations***"
  - Geostationary Operational Environmental Satellite (GOES)
  - Aerosol Optical Depth from the GOES Advanced Baseline Imager
  - Geographic Weighted Regression (GWR) against AirNow
  - Deep Neural Network Corrected (Sayeed et al *in prep*)



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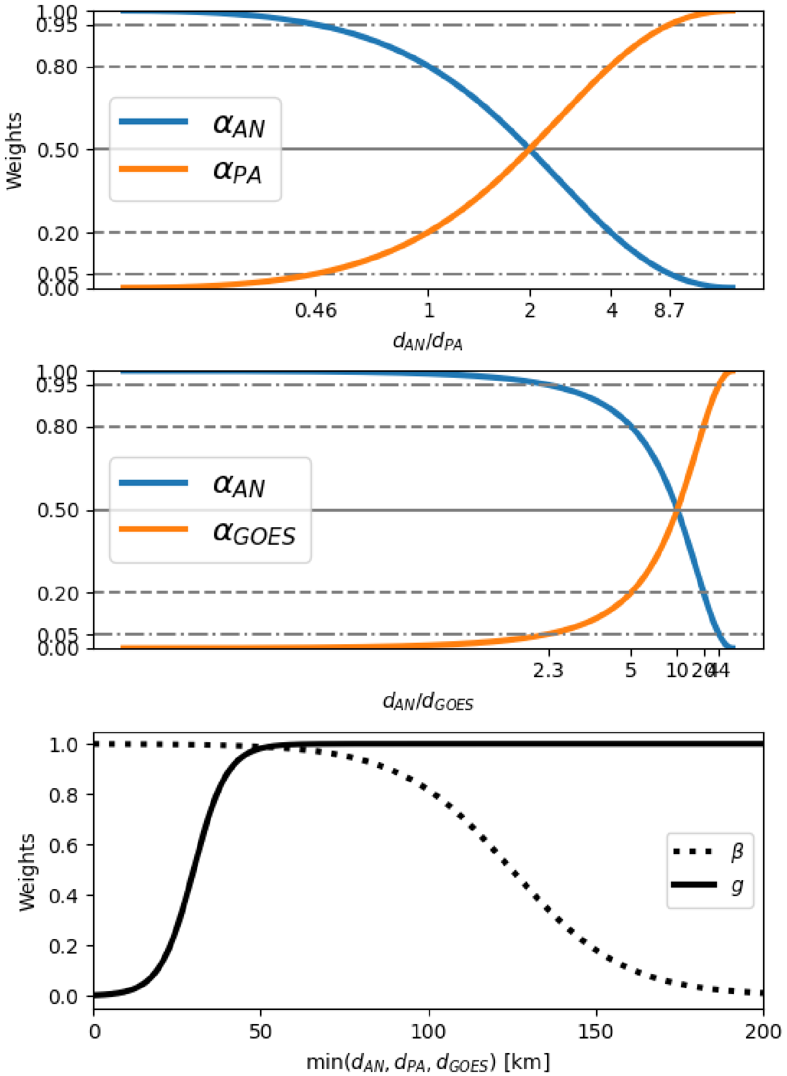
**Piece-wise regression as in Fire and Smoke Map

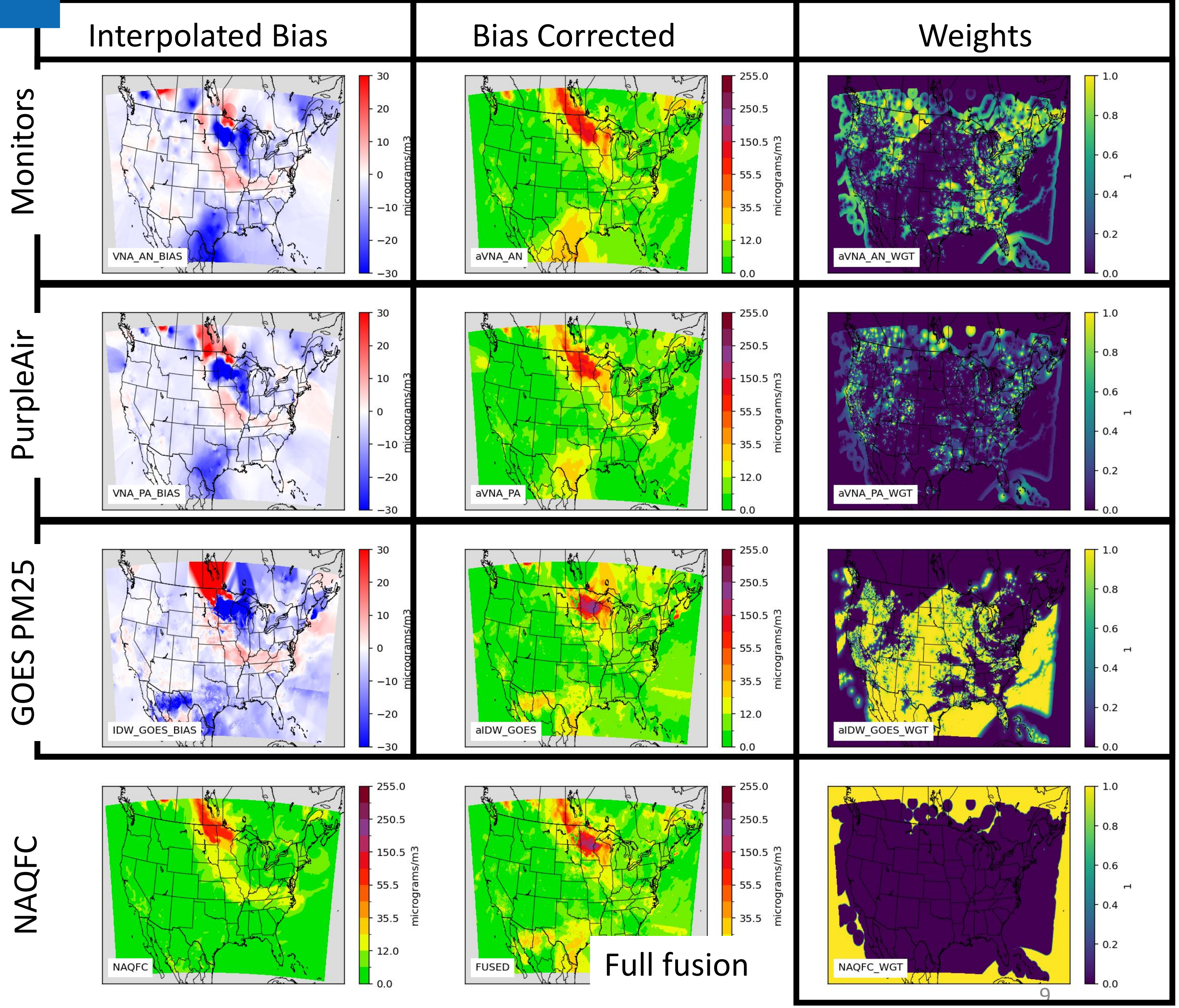
Ensemble Averaging Method

- Simple fusion of bias corrected surfaces
  - NAQFC, AirNow, PurpleAir, GOES-PM25
  - Fuse the surfaces based on distance
  - Apply different weights to ensembles
- $Y_{AN,PA,GOES} = \alpha_{AN} Y_{AN} + \alpha_{PA} Y_{PA} + \alpha_{GOES} Y_{GOES}$
  - $\alpha'_{AN} = (1 \times d_{AN})^{-2}$
  - $\alpha'_{PA} = (2 \times d_{PA})^{-2}$
  - $\alpha'_{GOES} = (10 \times d_{GOES})^{-2}$
  - $\alpha'_{tot} = \alpha'_{AN} + \alpha'_{PA} + \alpha'_{GOES}$
  - Normalize them all: $\alpha_i = \alpha'_i / \alpha'_{tot}$
- $Y_{AN,PA,GOES} = \beta \times Y_{AN,PA,GOES} + (1 - \beta) \times Y_{NAQFC}$

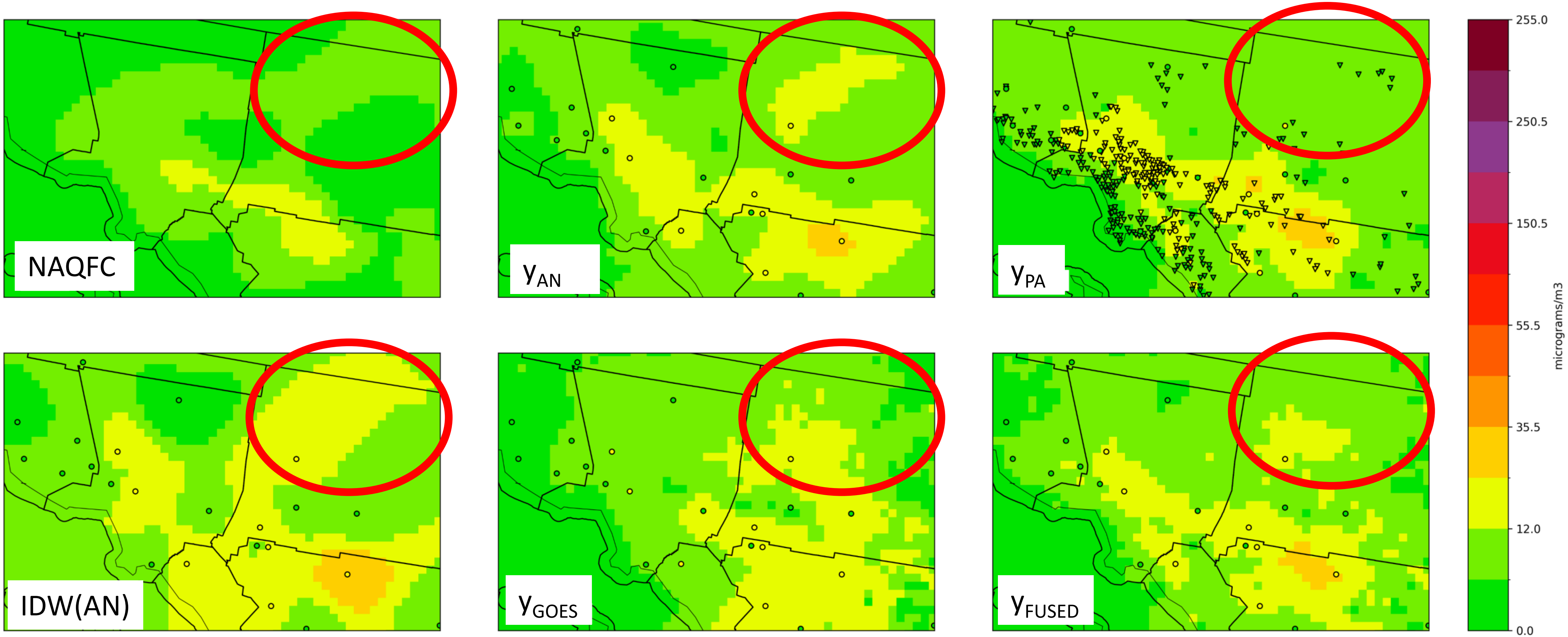


Case Study 2023-06-14T17Z

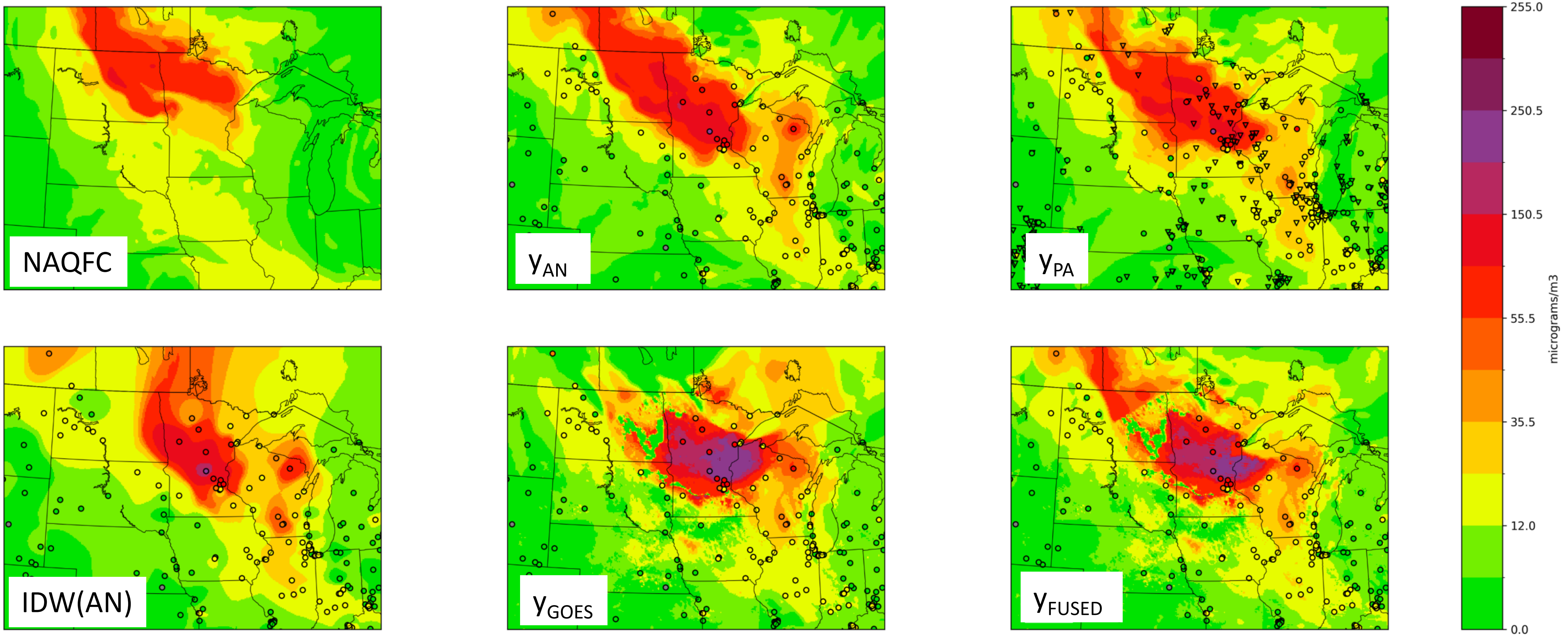
- Fairly typical day June day in the southwestern domain.
- Large fire contributions in Canada and sweeping down through Minnesota, Wisconsin and further
- 4 data sources
  - AirNow Monitors (top)
  - PurpleAir sensors
  - GOES PM25
  - NAQFC (bottom)
- Estimates
- Bias Corrections
- Full fusion



Los Angeles: 2023-06-14T17Z



Canadian Wildfires: 2023-06-14T17Z



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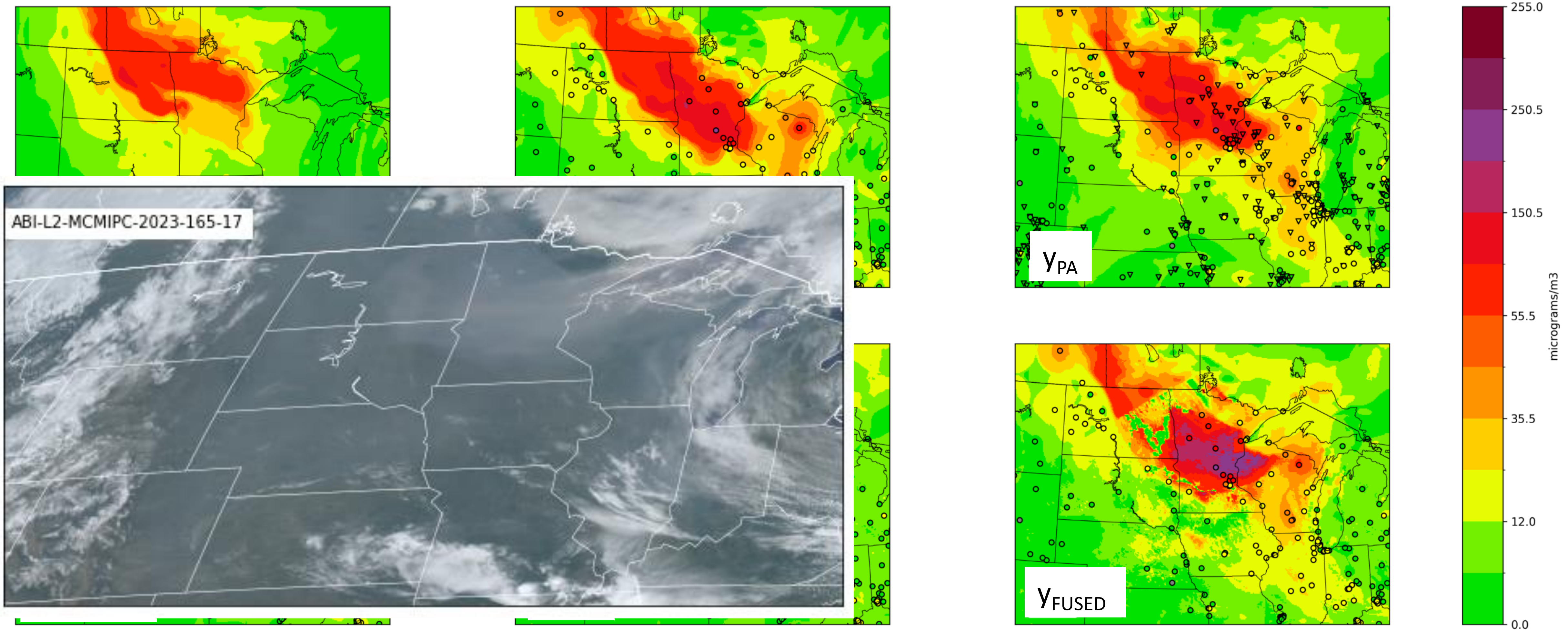

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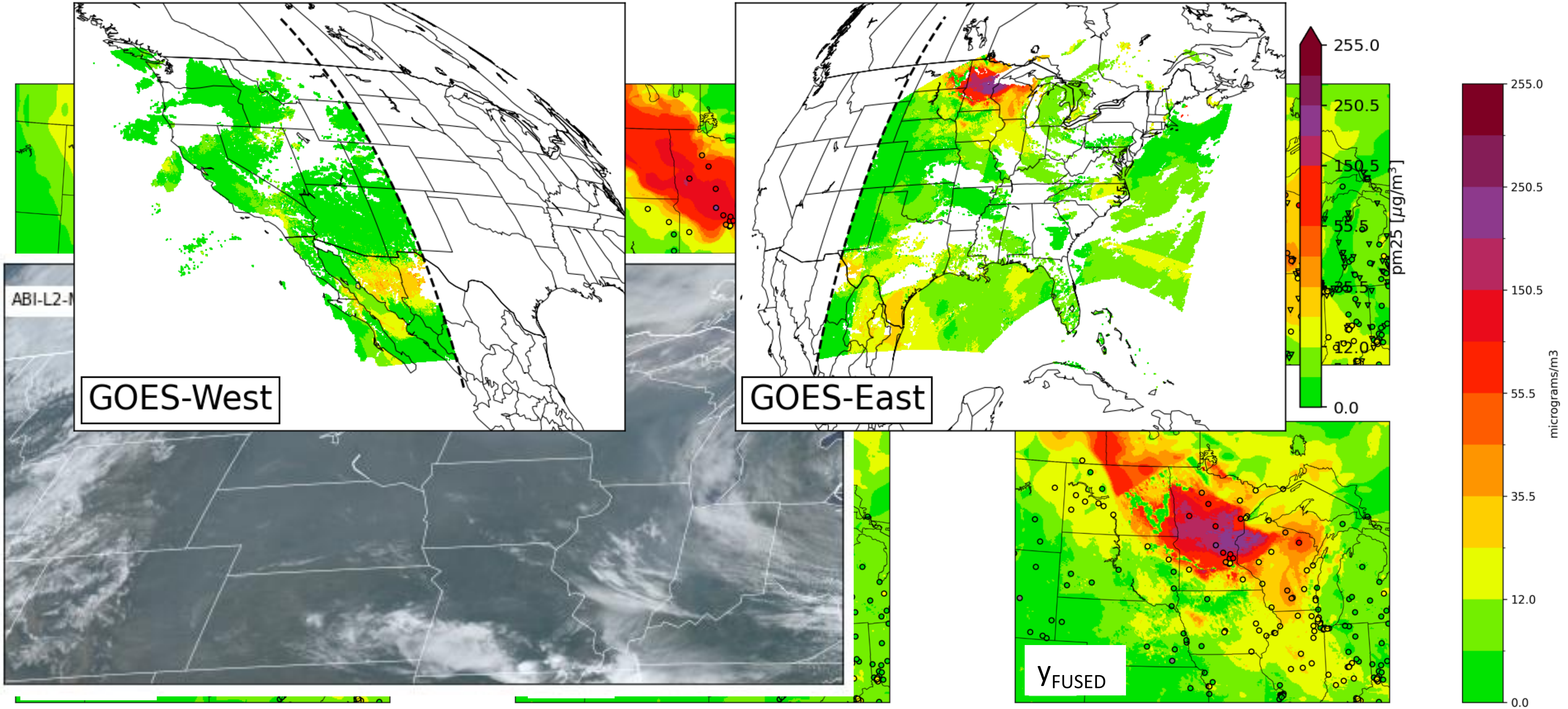
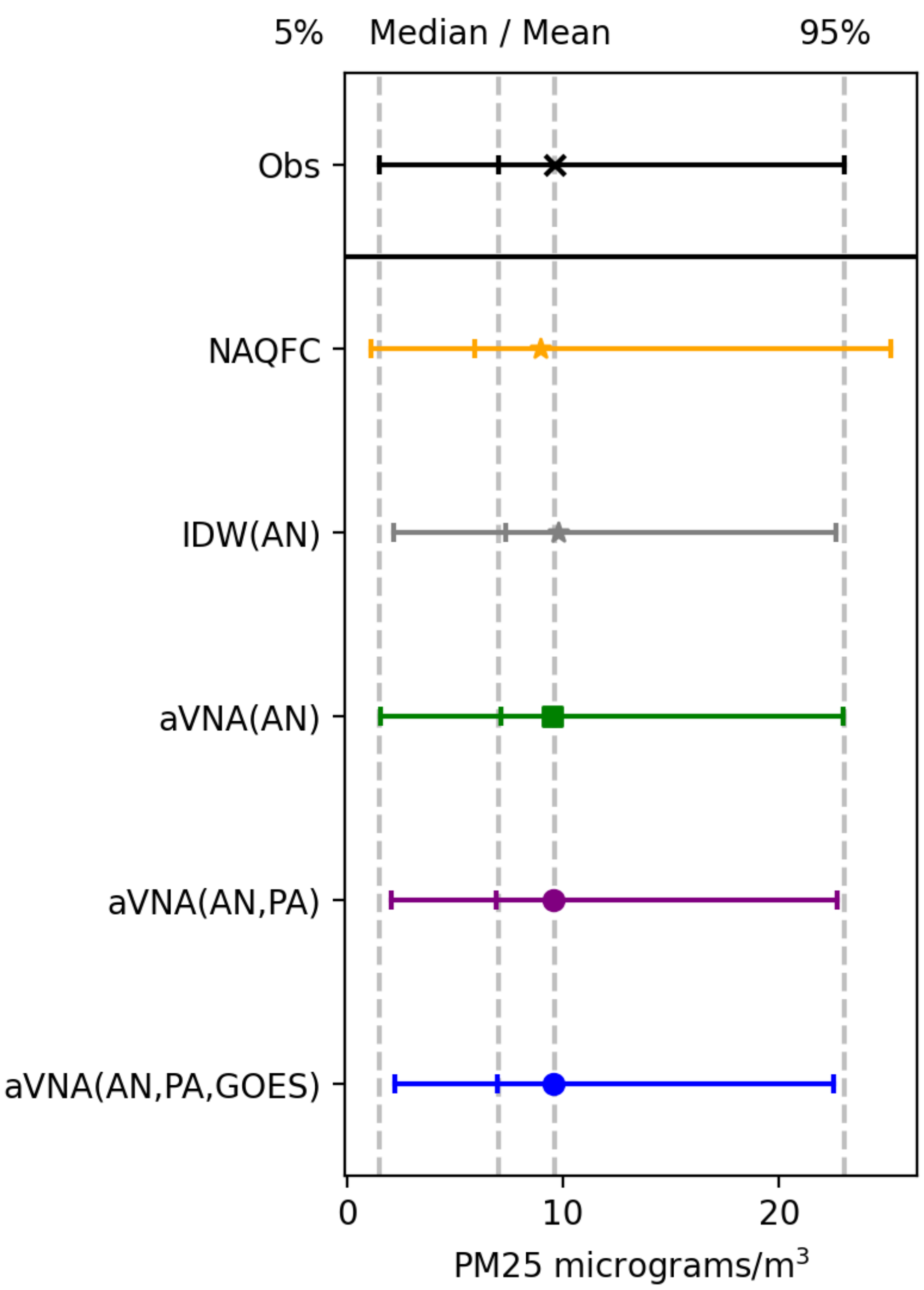


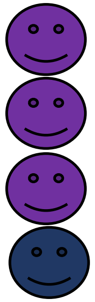
Evaluating the approach

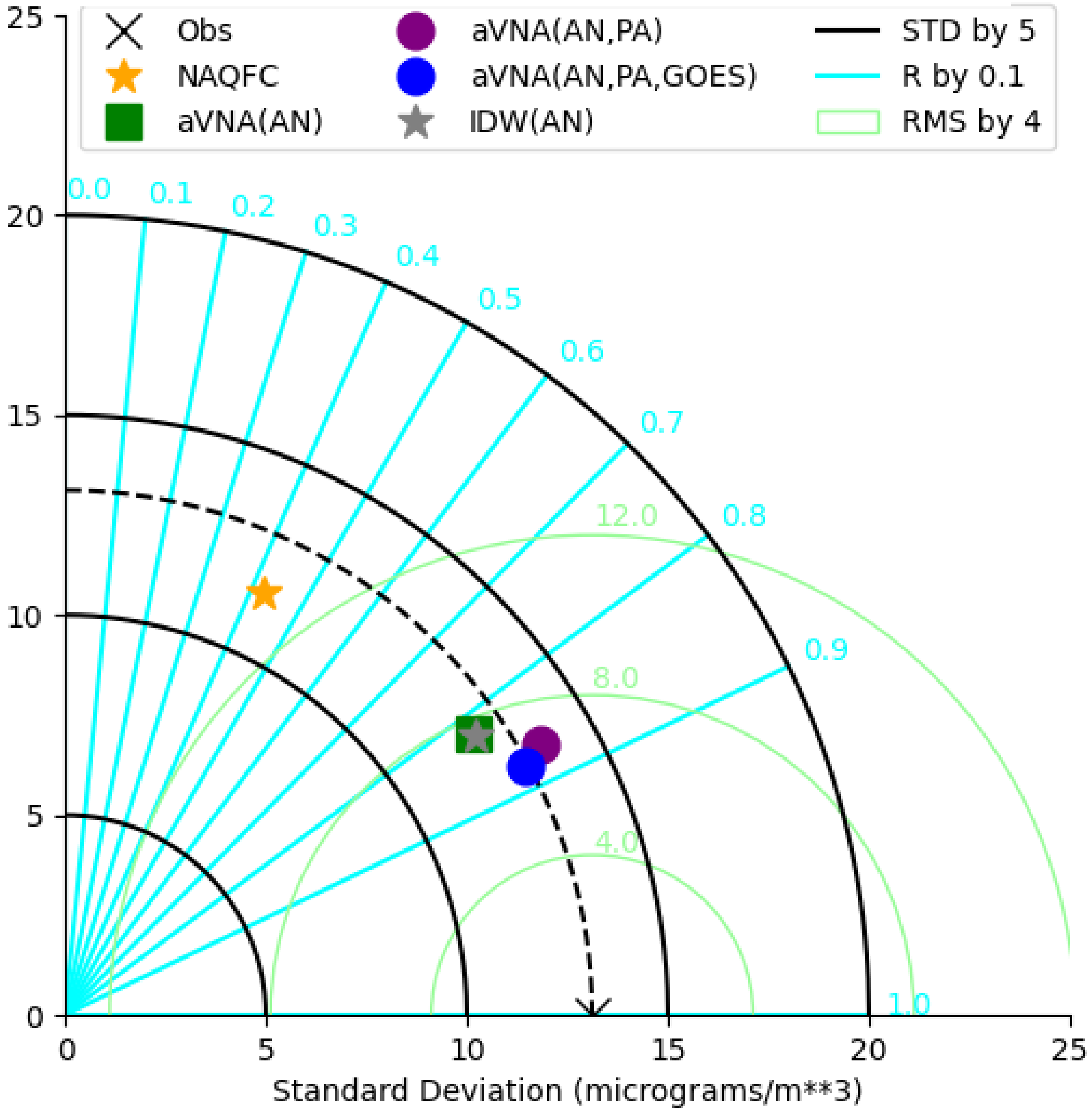
- That was just one hour…
- Applied daylight from Jun 2023 to Sept 2023
  - IDW as in AirNow (*)
  - NAQFC from NOAA (*)
  - Corrected w/ AirNow: AN
  - Correction w/ AN and PurpleAir: AN+PA
  - Correction w/ AN, PA and GOES: AN+PA+GOES
- Predicted each AirNow monitor without that monitor in the fusion
  - n=1.3M = 12 h/d * 30 d/m * 3.75m * 1000 /h
- Statistics: Normalized Mean Bias, Normalized Mean Error, RMSE, Correlation.



Performance Summary: June-Sept 2023 (daylight hours; n=1.3M)

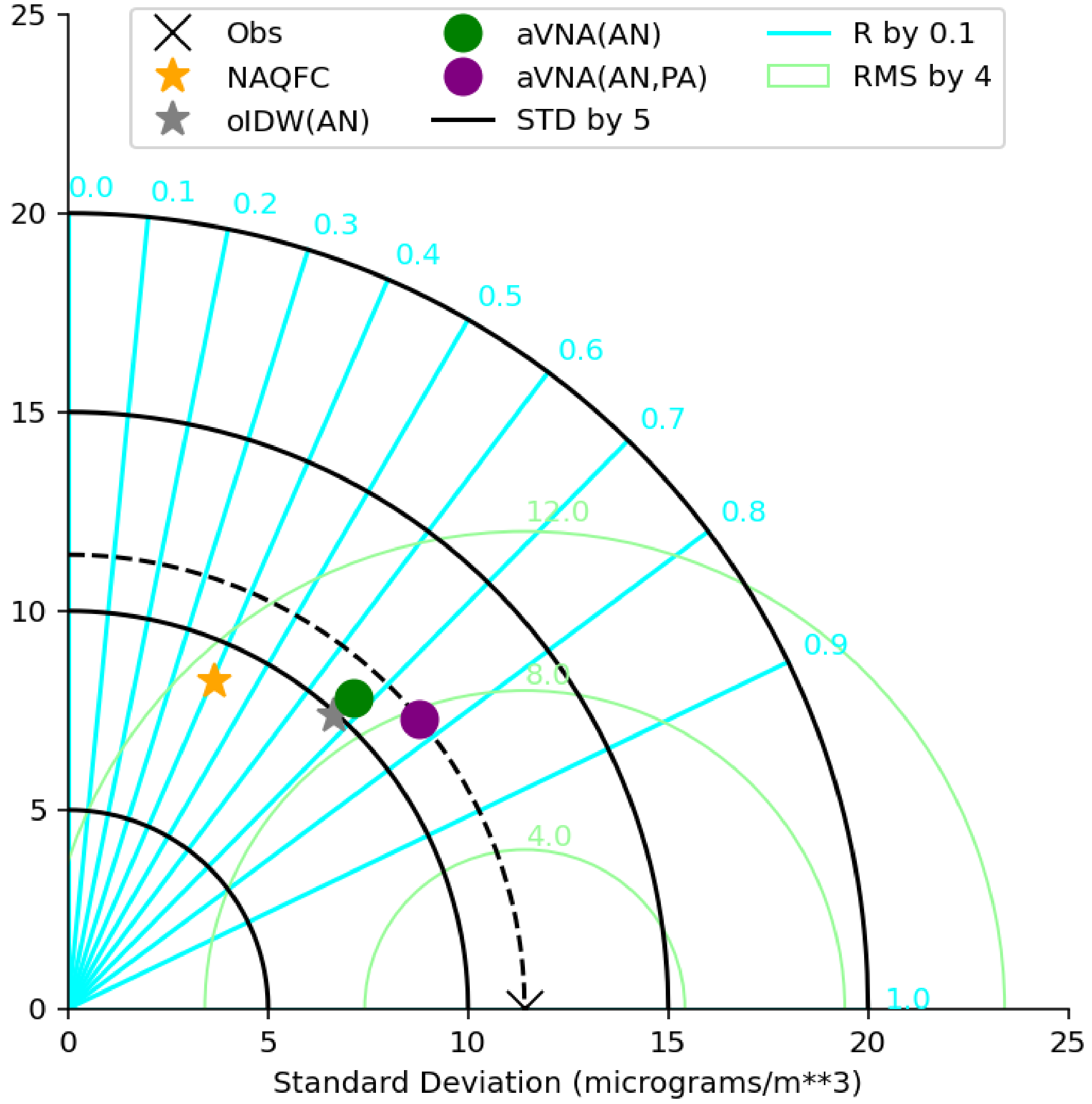
- Multiple statistics matter
  - Pearson correlation (y-axis)
  - centered Root Mean Squared Error (x-axis)
  - Reproduction of standard deviation
- The NAQFC has the lowest correlation, the highest RMSE, and the worst standard deviation.
- The AirNow and IDW have similar correlation, AirNow has better standard deviation.
- The fusion with PurpleAir improves standard deviation, correlation, and root mean squared error.
- The fusion with GOES is even better.





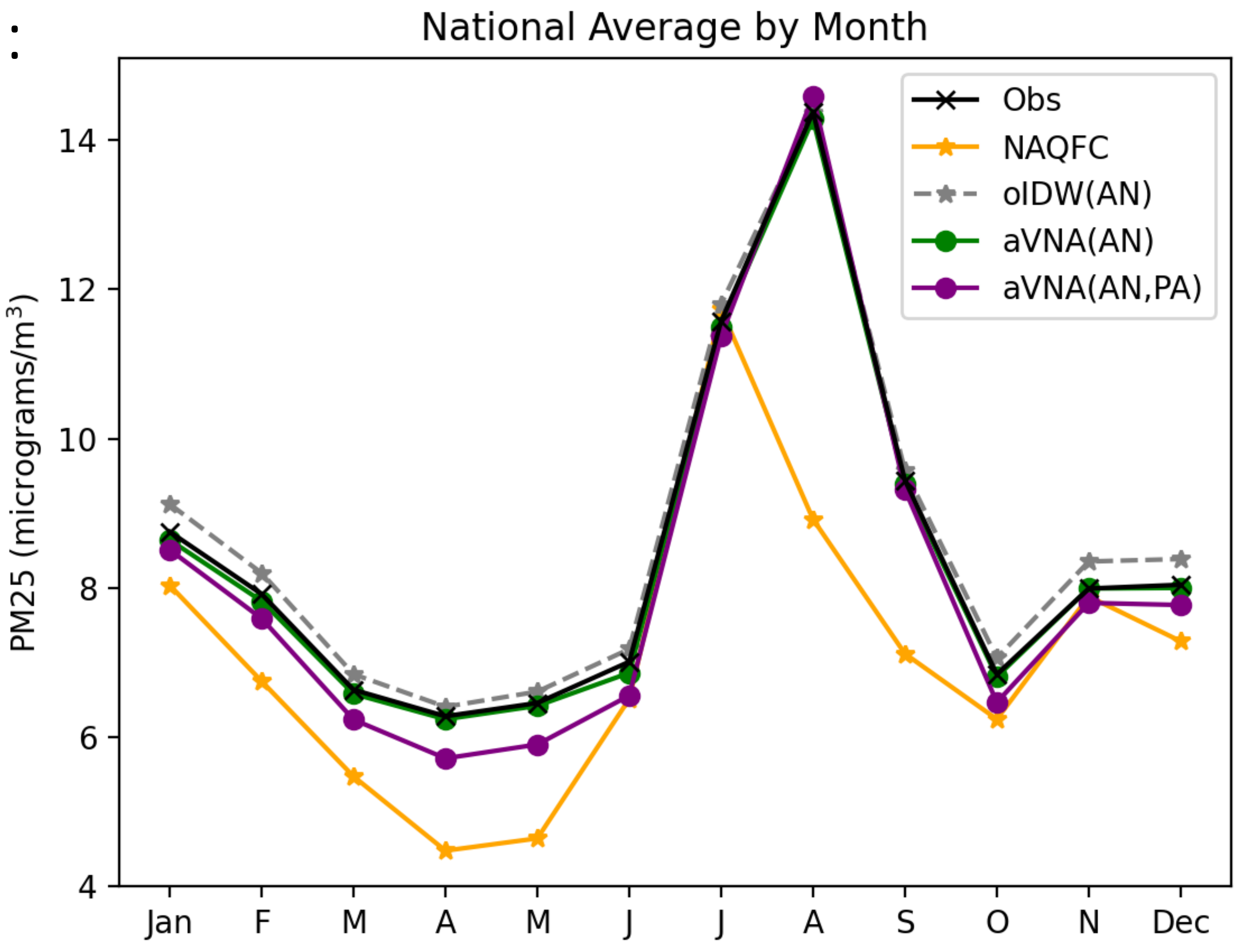
Performance Summary: June 2021-June 2022 (All hours; n=8M)

- Multiple statistics matter
  - Pearson correlation (y-axis)
  - centered Root Mean Squared Error (x-axis)
  - Reproduction of standard deviation
- The NAQFC has the lowest correlation, the highest RMSE, and the worst standard deviation.
- The AirNow and IDW have similar correlation, AirNow has better standard deviation.
- The fusion with PurpleAir improves standard deviation, correlation, and root mean squared error.
- Is the story more complex? When does one fail and the other succeeds?



Leave-1-out Validation: National Average of Predictions

- This figure summarizes the concentration of PM2.5 over the months of the year by method.
- All methods peak during the fire season with the NAQFC peaking during July.
- Whereas the observations and other methods all peak during August.
- Remember, this is validation. In application, the prediction at the monitor is equal to the monitor.



Leave-1-out Validation: National Correlation

- Incorporating PA improves the correlation especially during the fire season.
- aVNA(AN) has lowest correlation overall.
- aVNA(AN,PA) improves the correlation over the time of day.
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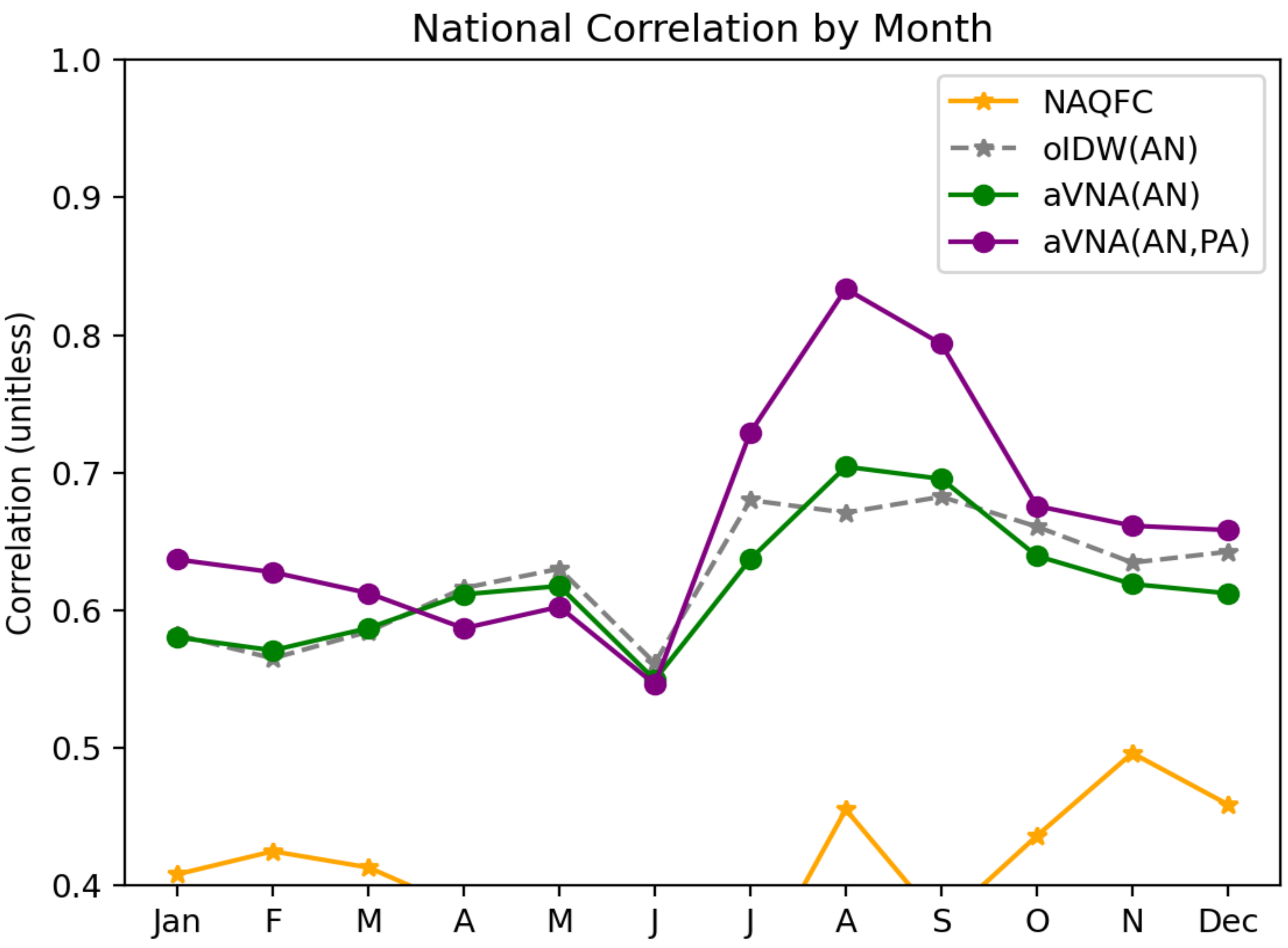

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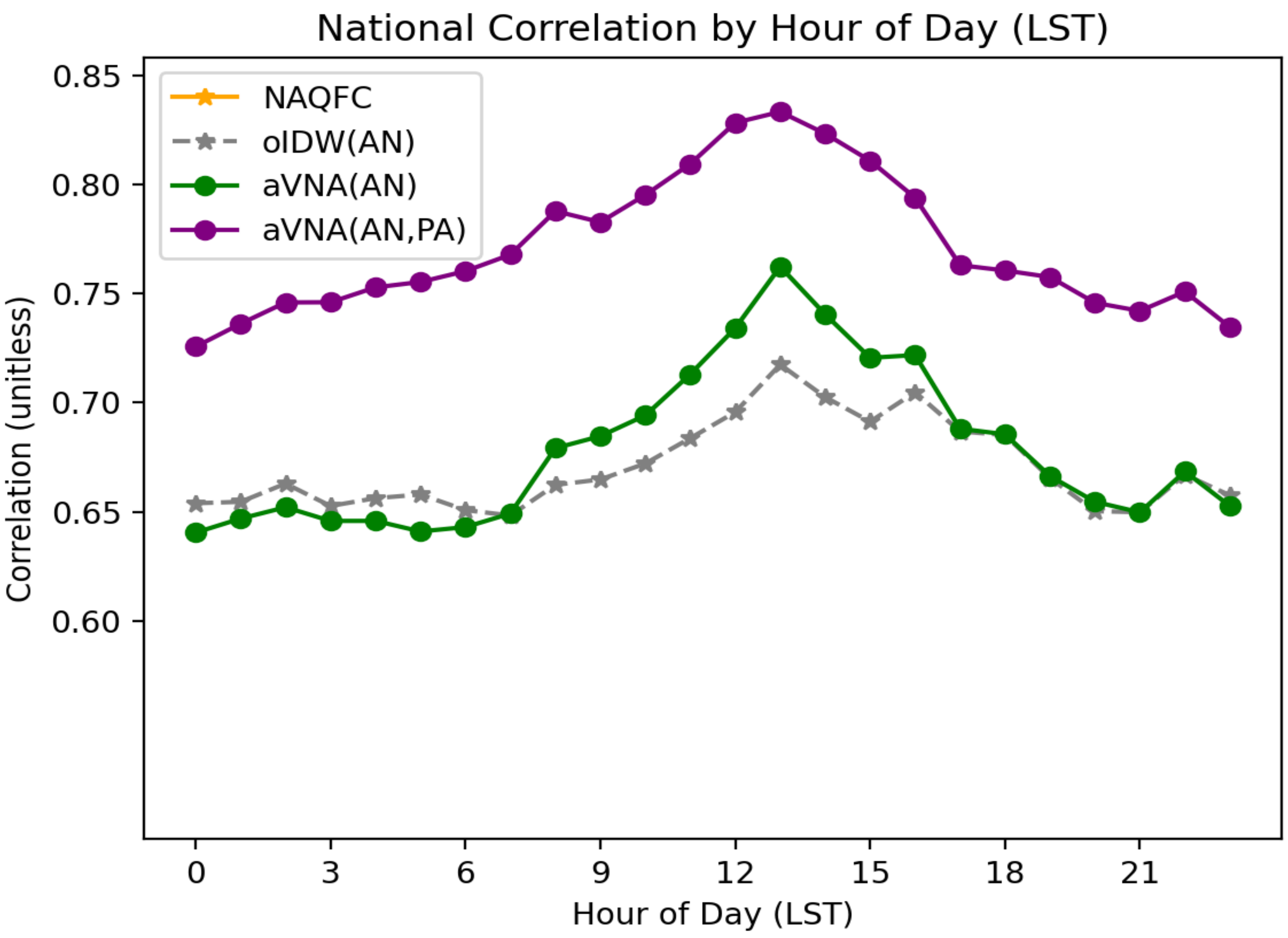
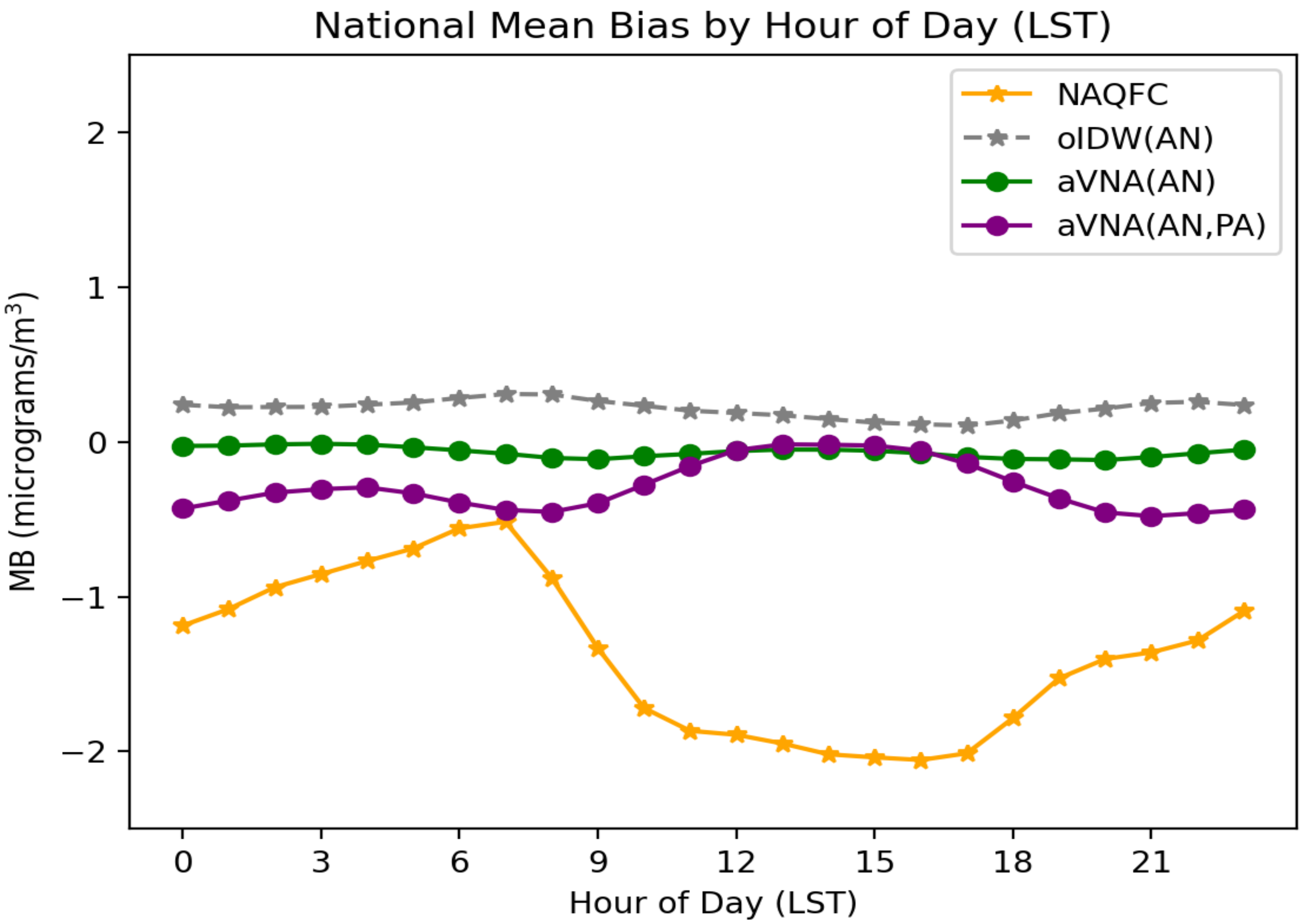


Leave-1-out Validation: National Mean Bias

- oIDW and aVNA(AN) have the most consistent bias.
- aVNA(AN,PA) has highest bias at night but is still quite good.
  - Currently, we use a single bias correction for PurpleAir.
  - Humidity varies with time of day and may need more complex correction.
  - Also, FEM technologies are evaluated most strictly for daily average concentration.
- Remember, this is validation. In application, the prediction at the monitor is equal to the monitor.



Summary

- AirNow needs an updated interpolation method.
  - EPA has long used models and statistical fusion to fill gaps with regulatory but has not incorporated these methods into AirNow.
  - Schulte et al. demonstrated including models and PurpleAir improved on simple interpolations and applied it in an AirNow-like system.
  - HAQAST Tiger Team evaluated GOES PM25 for real-time-applications.
- Fusion with PurpleAir is ready.
  - Discontinuities are less stark because datasets are more spatially consistent.
  - Value of PurpleAir is obvious because they are dense near monitors.
- Fusion with GOES PM25 ongoing work
  - HAQAST Tiger Team 2021 (Gupta) – now 2023 (Yang Liu)
  - Conceptually, the satellite value is highest away from monitors and sensors… making it hard to evaluate
  - ~5% of monitors are further than 30km from their nearest withheld monitor…

Questions?

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Extra Slides

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Evaluating the approach

- That was just one hour…
- Applied hourly data from Jun 2021 to Jun 2022
  - IDW as in AirNow (*)
  - NAQFC from NOAA (*)
  - Corrected w/ AirNow: AN
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  - ~~Correction w/ AN, PA and GOES: AN+PA+GOES~~
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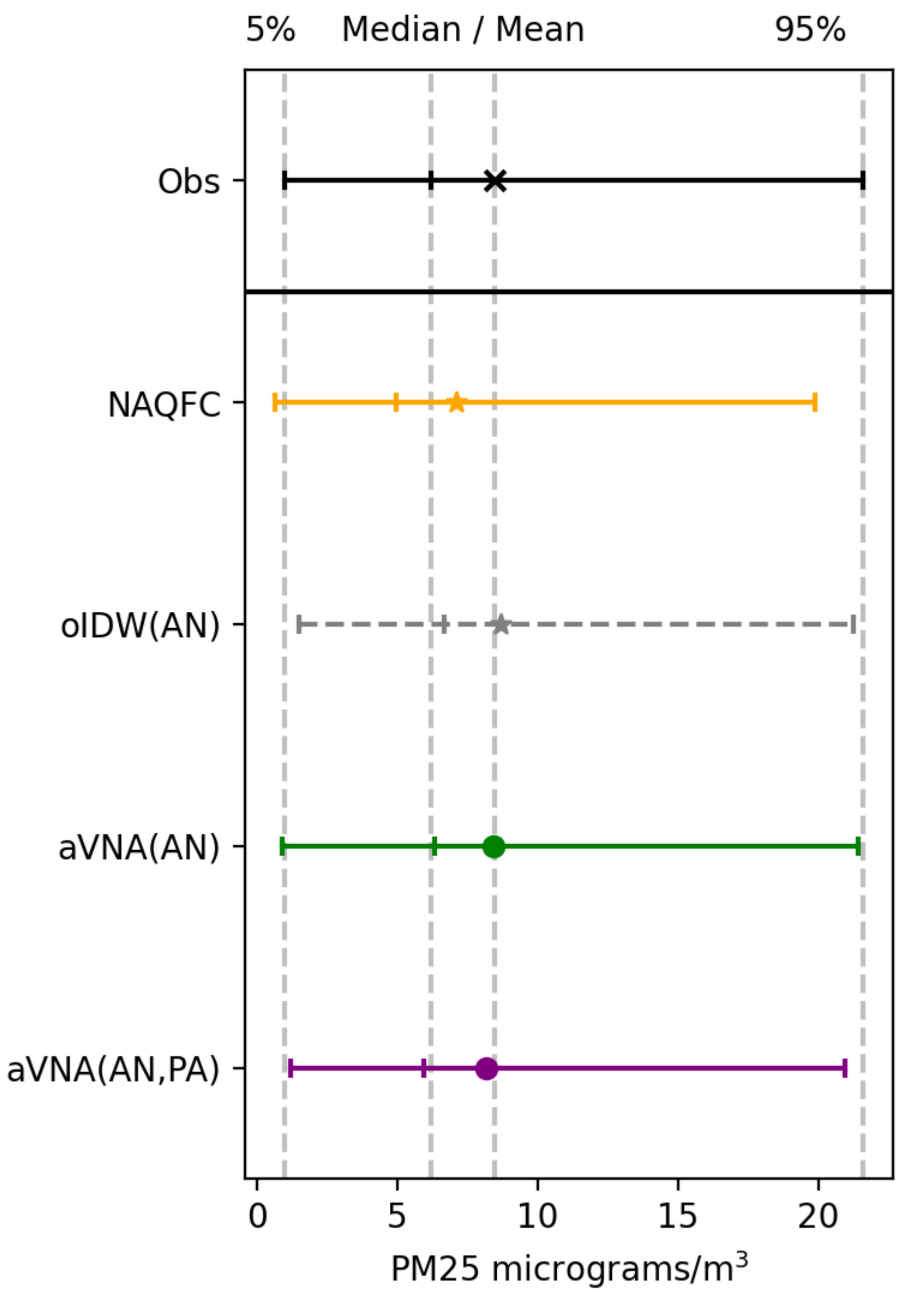
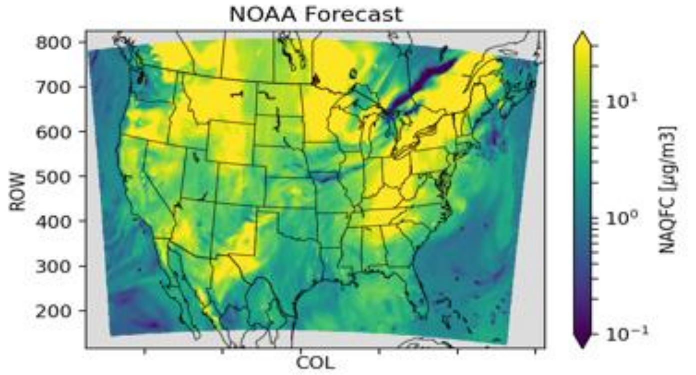
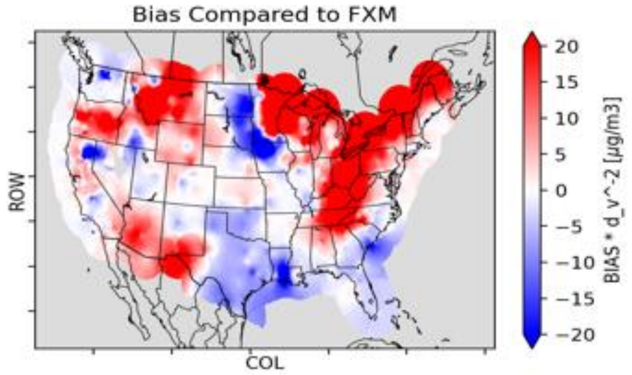
  - n=8M = 8760 h/y * 1000 /h
- Statistics: Normalized Mean Bias, Normalized Mean Error, RMSE, Correlation.

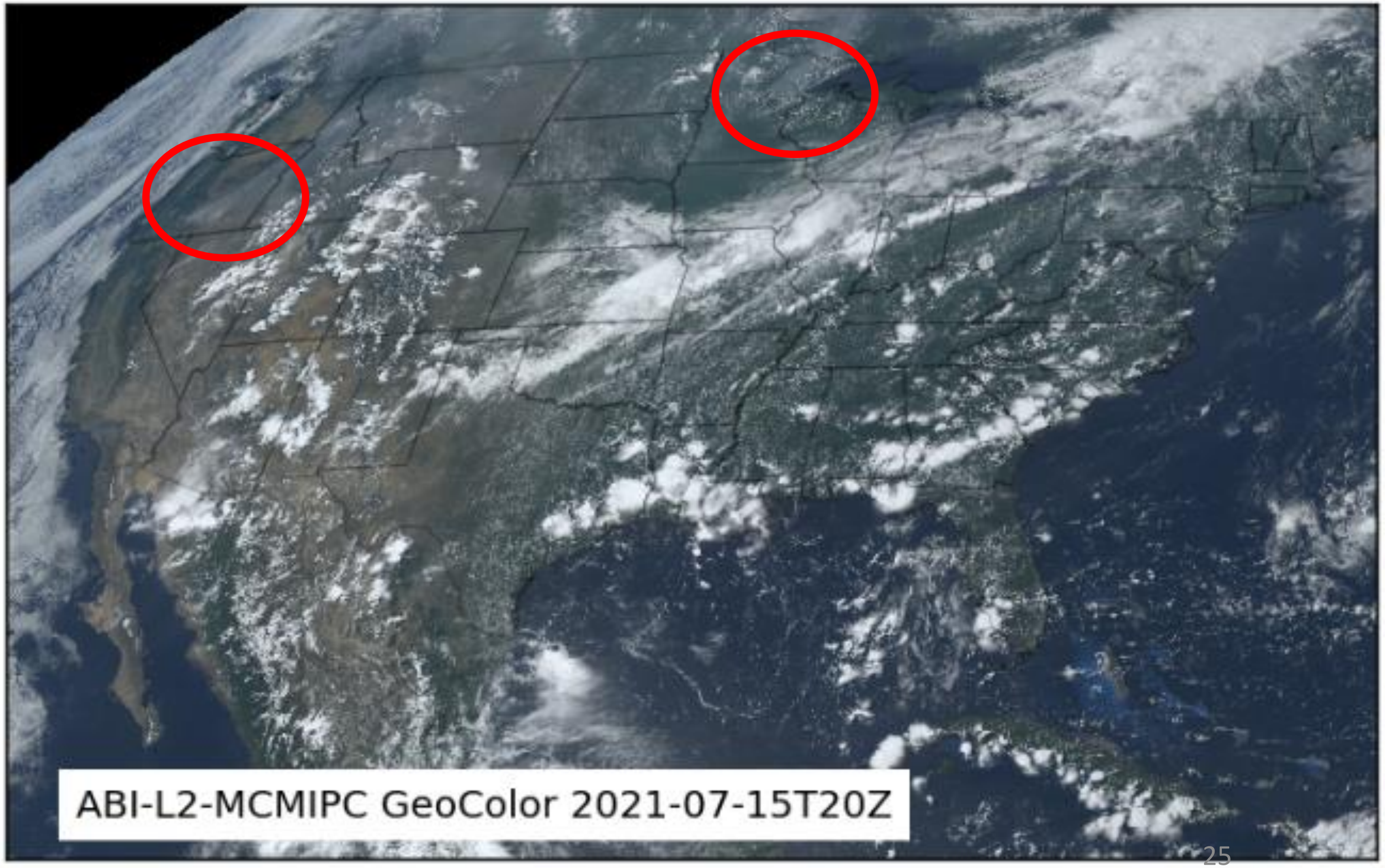


Fires are challenge any method

- IDW miss fires between stations.
- NAQFC had “persistent” fire emissions.
    - A fire continues to emit until it is observed to have stopped.
    - Not great at fires in the first place.
- Satellite imagery shows some smoke over high biased reasons.







EPA National-scale Approaches

- AirNow application at the national scale requires a speed, accuracy, and simplicity
- EPA has several techniques like residual kriging used by South Coast's.
  - Voronoi Neighbor Averaging (VNA), Extended VNA (eVNA)
  - Today, there will be a focus on a variation of eVNA that is additive VNA (aVNA)

Equation and Applications	Pros	Cons
$IDW = sum(O_n \times w_n)$ - AirNow	• Super Fast and Easy • Equals monitor!	• No causal mechanism.
Downscaler = f(M, O, N) - REA and CDC PHASE	• Rigor • Confidence intervals	• Too slow for this application
$eVNA = M \times sum(O_n / M_n \times w_n)$ - SIPs and RIA	• Fast • Equals monitor!	• Requires model* • Ratio can become unstable
$aVNA = M - sum((M_n - O_n) \times w_n)$ - ***new***, like Residual Kriging	• Fast • Equals monitor!	• Require model* • Can result in negative values

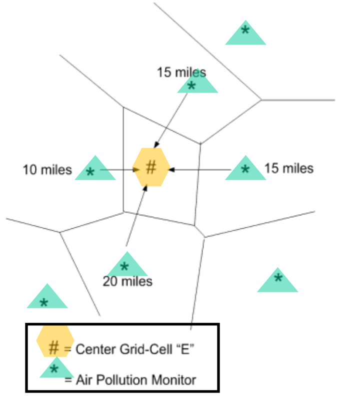
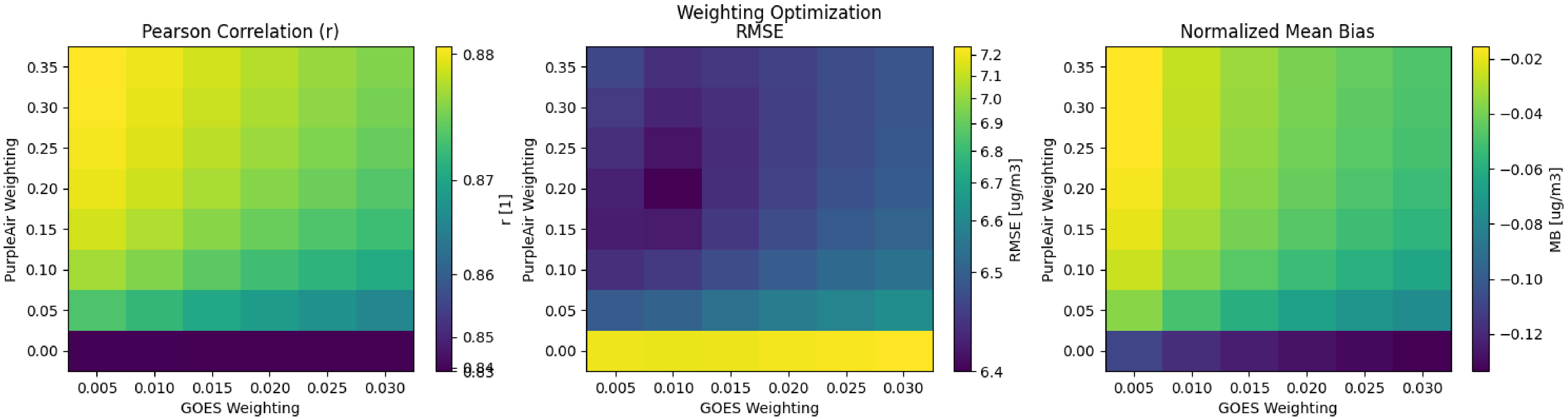


Figure courtesy of: Brian Timin

*Our NOAA colleagues make hourly forecasts twice a day!

- n = neighbors (AirNow=10-nearest; Otherwise=Voronoi)
- $w_n = d_n^p / sum(d_n^p)$: p = -2 or -5 in AirNow

Preliminary weighting figure.



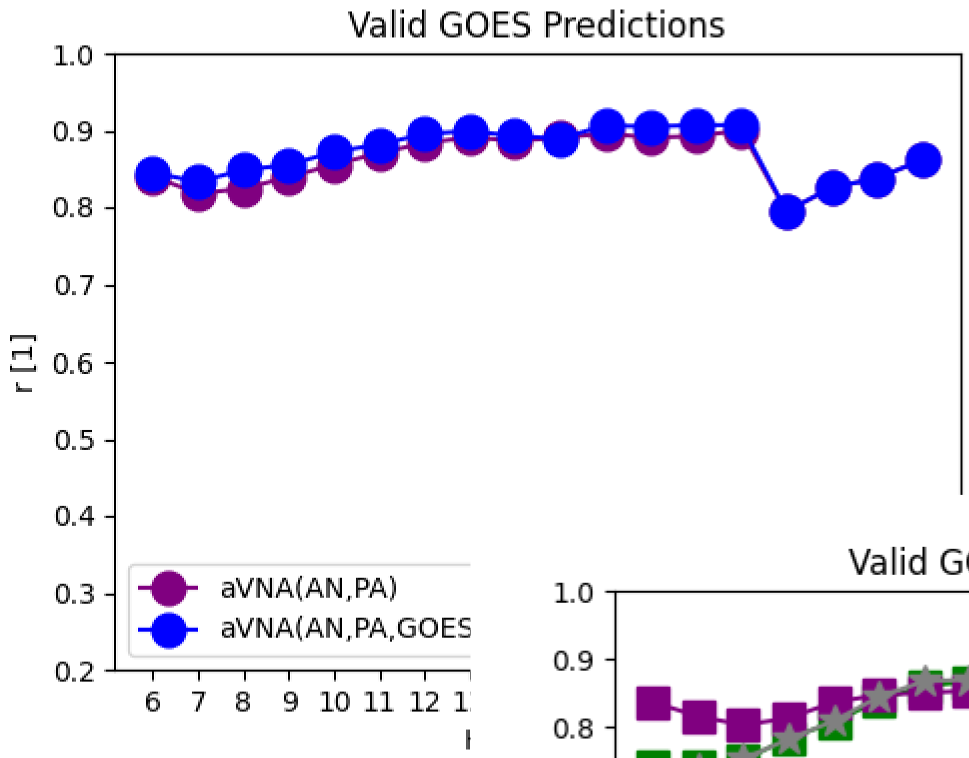
Alternative Ensemble Weighting Approaches

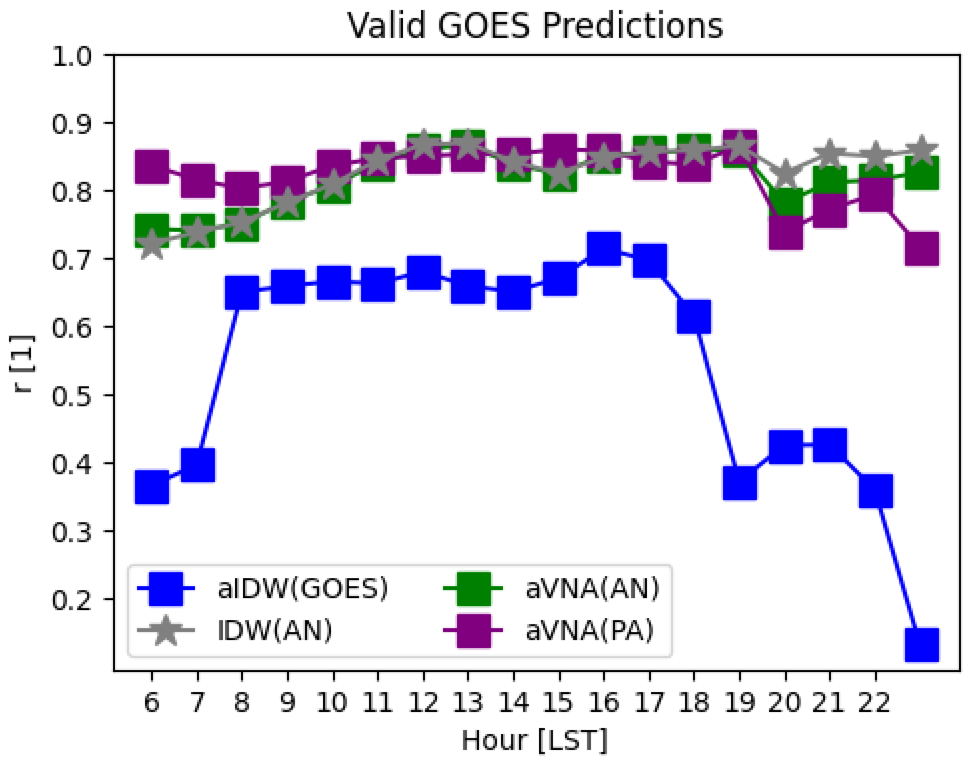
- We need a method to synthesize the products:
  - At this point, we have a potential of 4 fusion products
  - 2 bias correction methods (aVNA, eVNA), 2 data sources (AirNow, PurpleAir)
- Geographically Varying Weights (GVW)
  - Similar to Requia[1], but implemented like Skipper[2]
  - $Y_{fused} = \Sigma_i \alpha_i Y_i$
  - $\alpha_i = c_i + \beta_{i,0} x + \beta_{i,1} y + \beta_{i,2} d_{PA} + \beta_{i,2} d_{AN}$
  - c_i and all β are fit using least squares regression
- Random Forest Regression (RF)
  - Features: x, y, d_{PA}, d_{AN}, Y_i estimates from leave-one-out cross-validation
  - Configuration: Minimum 20 features for a split; 100 trees.
- **Not Shown**: Few day tests show
  - Both GVW and RF have better correlation than current approach; RF best.
  - But…. Current approach has better standard deviation than either
- This will likely need to be revisited when bringing in the GOES-PM25.

[1] Requia et al. https://pubs.acs.org/doi/10.1021/acs.est.0c01791
[2] Skipper et al. https://doi.org/10.1021/acs.est.0c08625

Leave-1-out Validation: National Mean Bias

- GOES shows structure in the bias that is associated with long-distance extrapolation…
- The fusion actually doesn't use those cells (too far away)
- Remember, this is validation. In application, the prediction at the monitor is equal to the monitor.

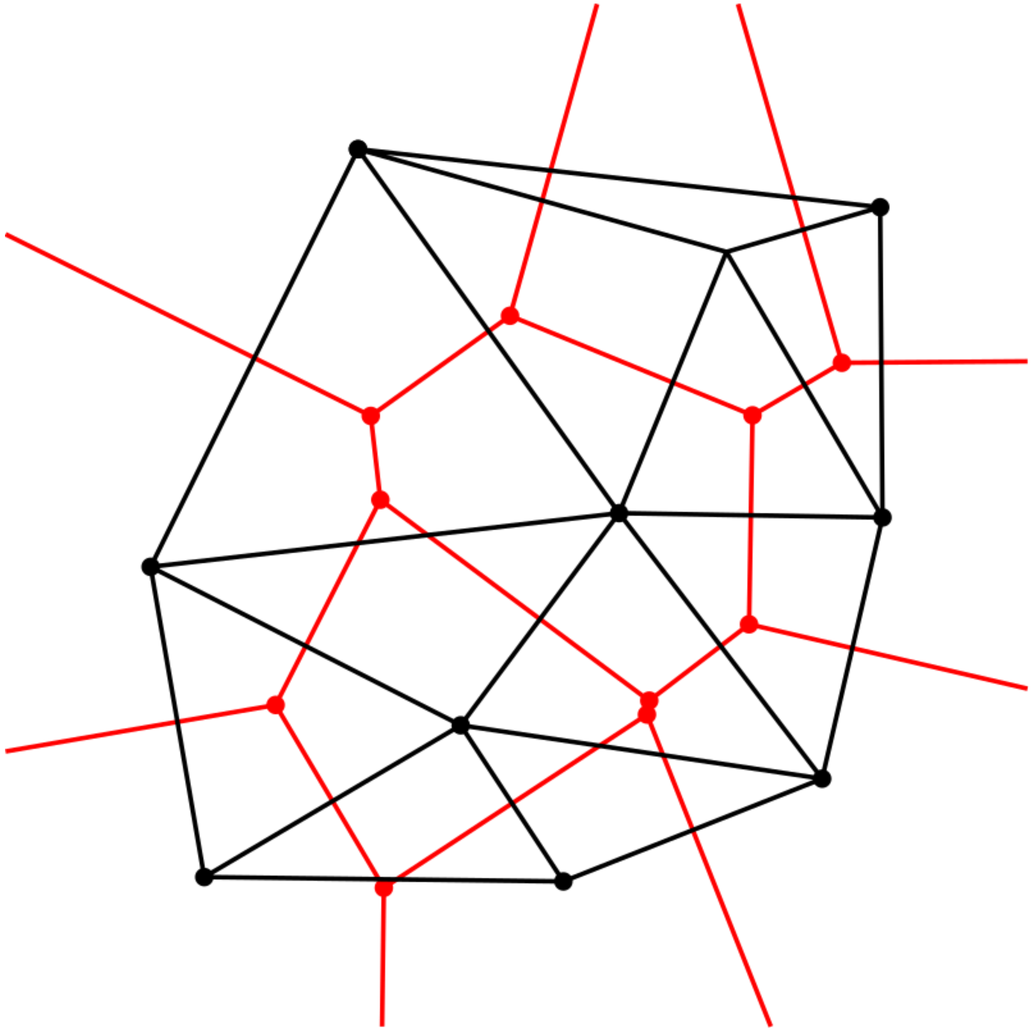




Supplement on eVNA

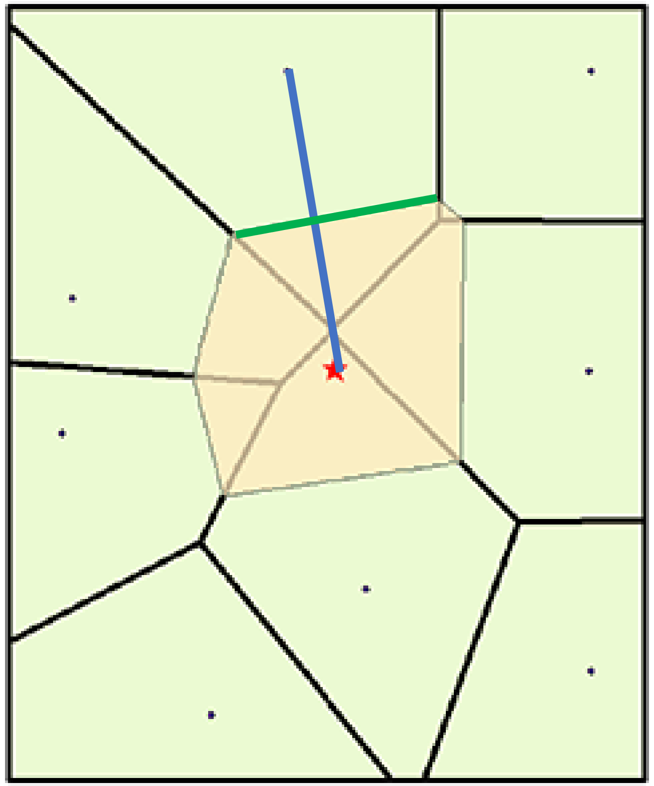
What is a Voronoi diagram and how does it relate to a Delaunay Tessellation?

- The Voronoi Diagram is show in red while the Delaunay Tessellation is in **black**
  - Red polygons show area where black lines delimit closest neighbor relationships
  - **Black triangles** are made by vertices where no triangle includes another's vertices
- Voronoi Diagram
  - Extend a radius in all directions from each black vertex.
  - When two vertices meet, stop.
  - This is the extent of the "area of influence"



Natural Neighbor Interpolation

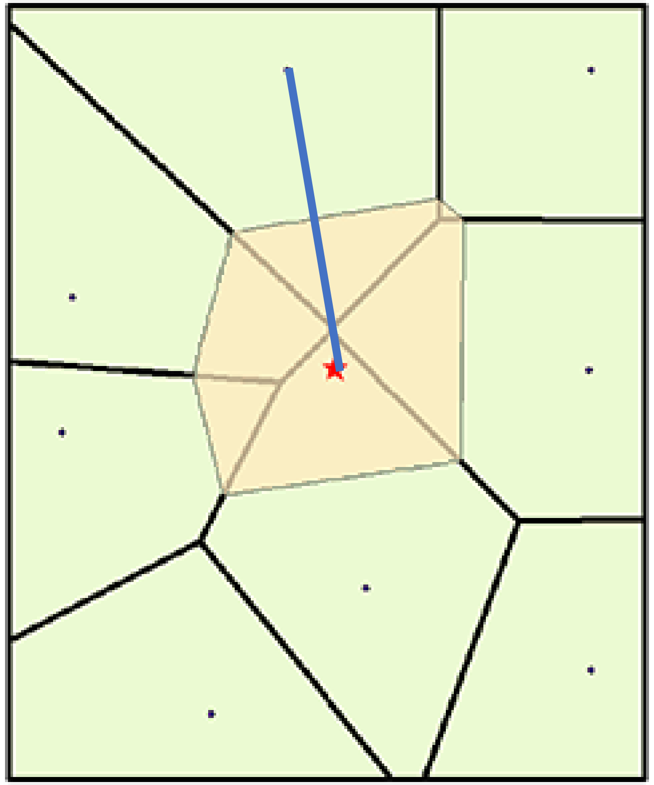
- Sibson published a method in 1981
- Create a complete Voronoi Diagram shown in black lines with green faces
- Add a point and redevelop a local polygon (yellow)
- Contribution Weights:
  - ***Sibson weights***: The area intersection between old polygons and the new polygon are the weights.
  - ***Laplace weights***: The neighbor's shared face length (green line) divided by the distance to the neighbor (blue line).
  - All normalized to 1.
- ***Sibson and Laplace weights*** use elements of the Voronoi polygon.



Sibson, R. "A Brief Description of Natural Neighbor Interpolation," chapter 2 in *Interpolating Multivariate Data*. New York: John Wiley & Sons, 1981. 21–36.

VNA is NNA without the Voronoi diagram

- First published in MATS User Guide (2007)
- Timin, Wesson, Thurman (2010)
- VNA in EPA Tools
  - Create a complete Voronoi Diagram shown in green and yellow
  - ***weights***: distance to the neighbor (blue line)
- So, VNA does not use any element of the Voronoi polygon… at all.
  - This is actually the Delaunay neighbor average weighed by *f*(distance)
  - Constructing a Delaunay diagram is twice as fast as Voronoi diagram.



Abt, MATS User Guide, 2007.. (2010).

Timin, Wesson, Thurman, Chapter 2.12 of *Air pollution modeling and its application XX*. (Eds. Steyn, D. G., & Rao, S. T.) Dordrecht: Springer Verlag.

What is extended VNA?

- VNA : $Y = \sum_i w_i x_i$
- eVNA is VNA with a special x_i
- eVNA : $Y = \sum_i w_i o_i \frac{m}{m_i}$
  - *o_i = observation at neighbor (i)*
  - *w_i = inverse distance squared*
  - *m/m_i* = model spatial gradient

- But wait, m is a constant…
- $Y = m \sum_i w_i \frac{o_i}{m_i}$; or $\mathrm{m}Y'$; $Y' = \sum_i w_i \frac{o_i}{m_i}$
  - *o_i/m_i* = relative model bias correction
  - So, this is just the interpolation of the inverse Normalized Bias.