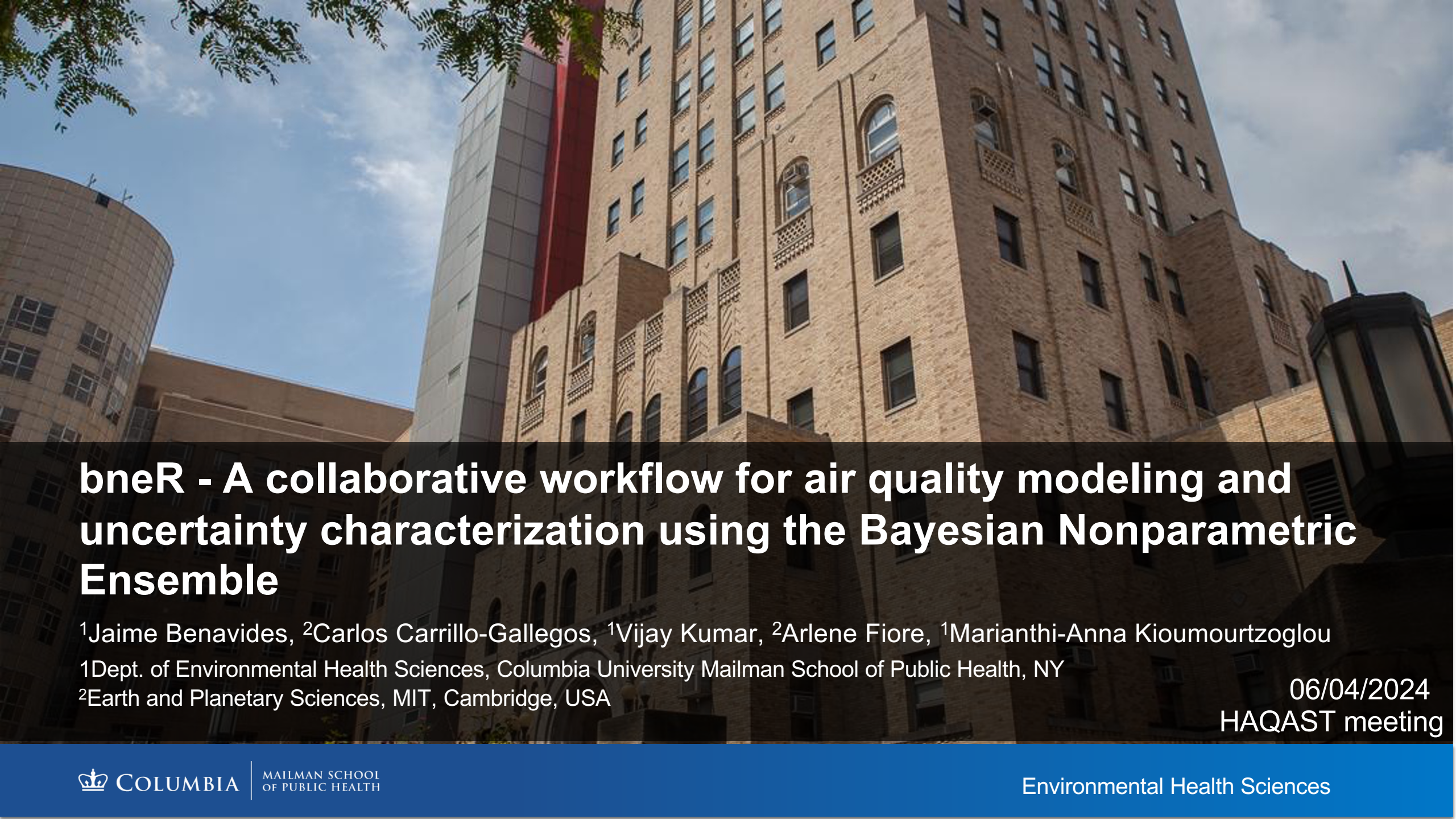




# **bneR - A collaborative workflow for air quality modeling and uncertainty characterization using the Bayesian Nonparametric Ensemble**

<sup>1</sup>Jaime Benavides, <sup>2</sup>Carlos Carrillo-Gallegos, <sup>1</sup>Vijay Kumar, <sup>2</sup>Arlene Fiore, <sup>1</sup>Marianthi-Anna Kioumourtzoglou

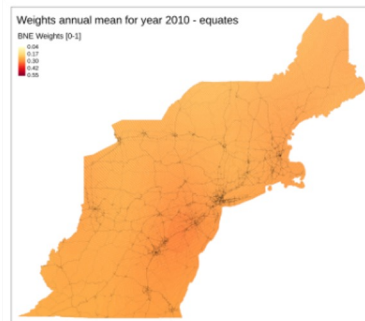
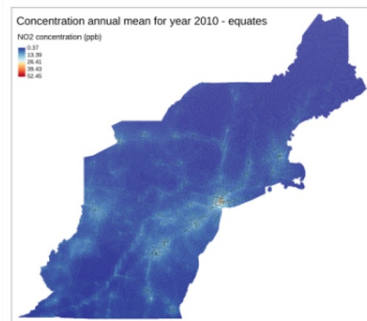
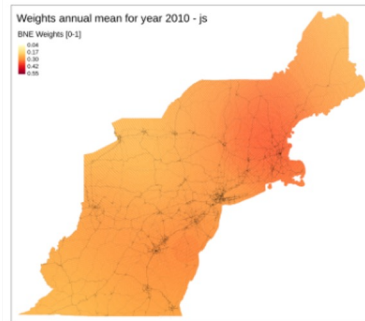
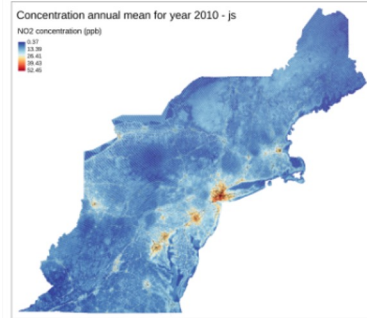
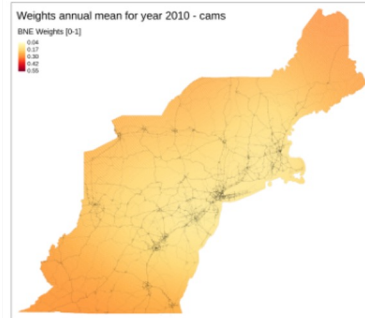
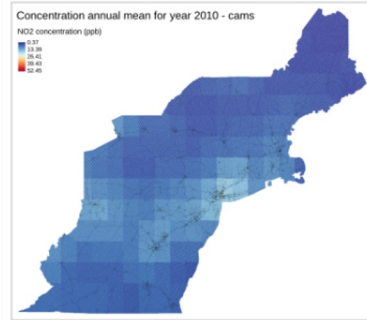
<sup>1</sup>Dept. of Environmental Health Sciences, Columbia University Mailman School of Public Health, NY

<sup>2</sup>Earth and Planetary Sciences, MIT, Cambridge, USA

06/04/2024  
HAQAST meeting

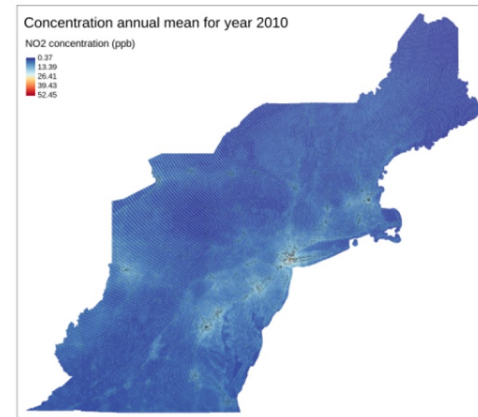


# Bayesian Nonparametric Ensemble (BNE)

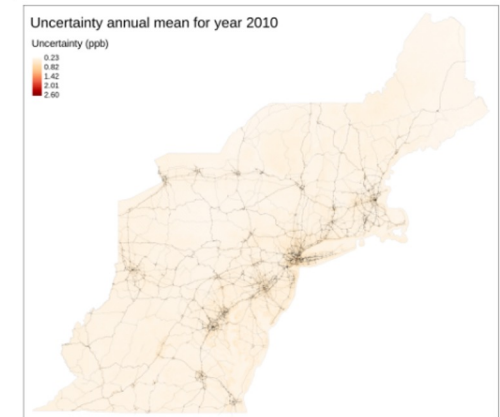


Input base models

Model weights [0-1]



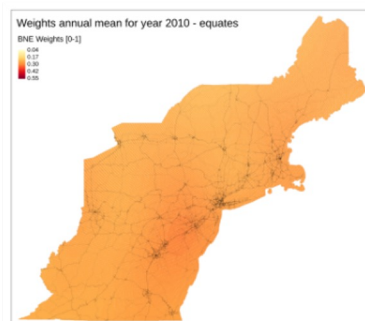
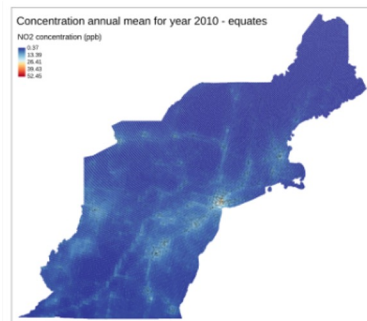
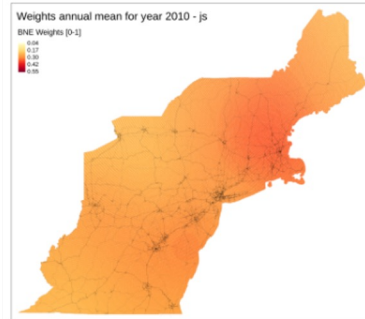
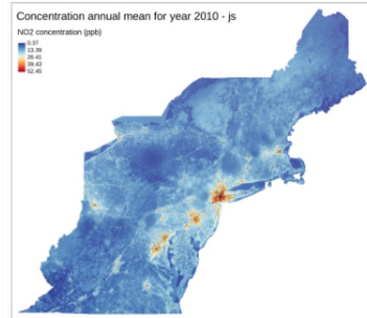
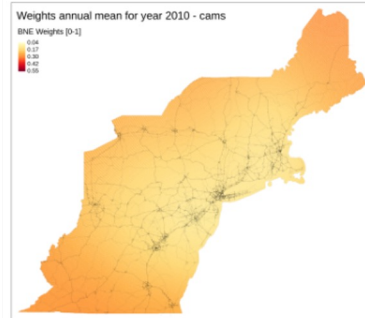
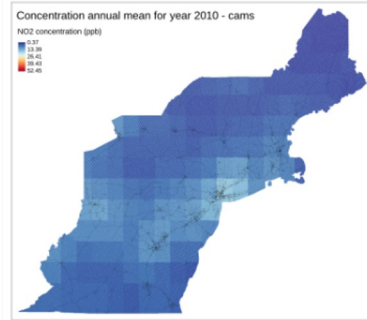
Ensemble concentrations



Uncertainty

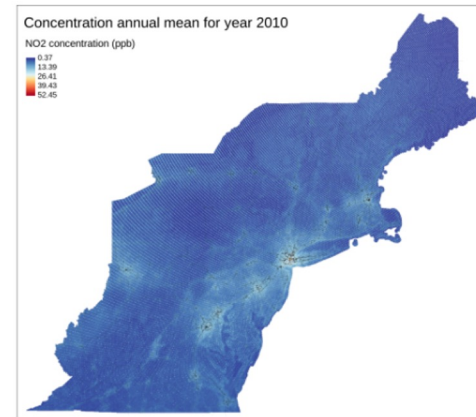


# Bayesian Nonparametric Ensemble (BNE)

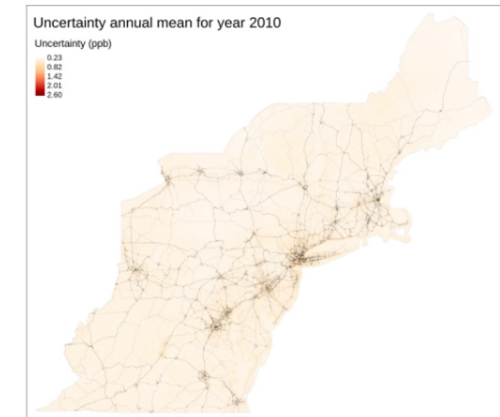


Input base models

Model weights [0-1]



Ensemble concentrations



Uncertainty

For some more details, please visit Vijay's Kumar poster on BNE!

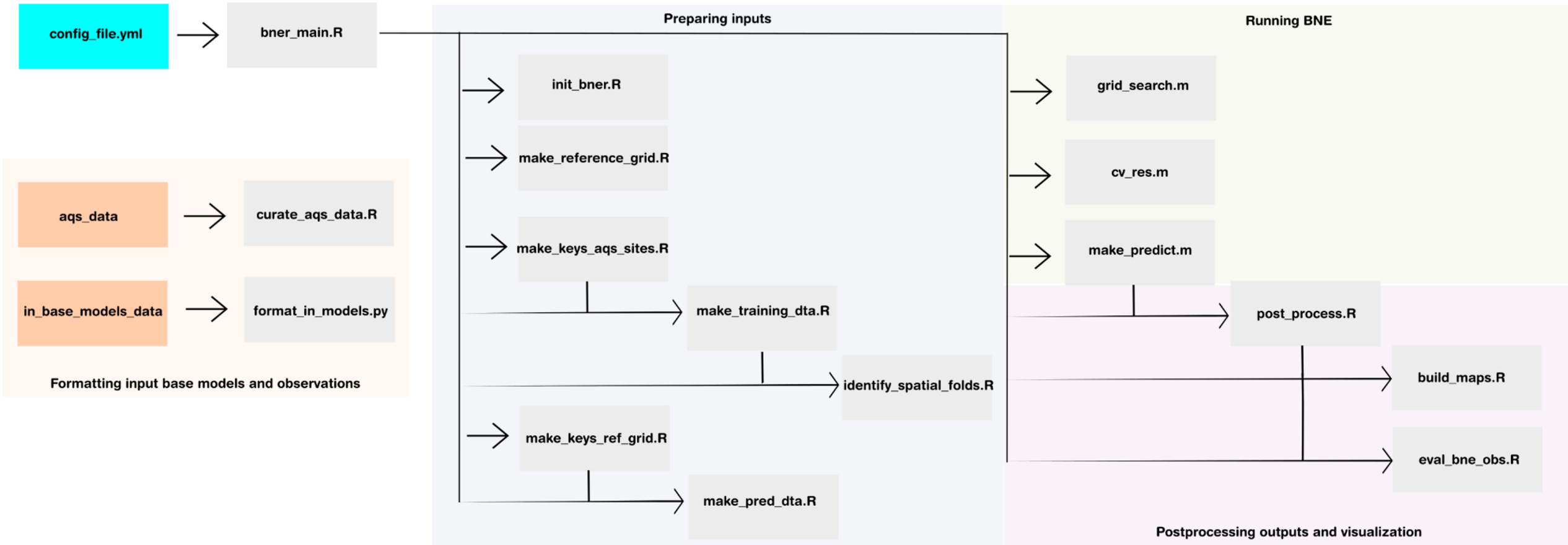


# Input base models

| Dataset                                                | Pollutants                                           | Spatial Resolution      | Spatial Coverage | Temporal Coverage | Methodology                                                                                                                                     |
|--------------------------------------------------------|------------------------------------------------------|-------------------------|------------------|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| CAMS<br>(ECMWF Atmospheric Composition Reanalysis 4)   | NO <sub>2</sub> , PM <sub>2.5</sub> , O <sub>3</sub> | 25x 25 km <sup>2</sup>  | Global           | 2002-2022         | Data assimilation using Integrated Forecast System (IFS) model for aerosols, chemistry, and greenhouse gasses, and several emissions datasets   |
| EQUATES<br>(EPA Air QUALity Time Series)               | NO <sub>2</sub> , PM <sub>2.5</sub> , O <sub>3</sub> | 12 x 12 km <sup>2</sup> | CONUS            | 2002-2019         | WRF 4.1.1, CMAQ 5.3.2, National Emissions Inventory 2017                                                                                        |
| FAQSD<br>(Fused Air Quality Surface Using Downscaling) | PM <sub>2.5</sub> , O <sub>3</sub>                   | 12 x 12 km <sup>2</sup> | Global           | 2002-2019         | Fusion of CMAQ chemical transport model with ground level AQS data                                                                              |
| JS<br>(Di et. al)                                      | NO <sub>2</sub> , PM <sub>2.5</sub> ,                | 1 x 1 km <sup>2</sup>   | CONUS            | 2000-2016         | Generalized additive model of three ML methods incorporating AQS data, AOD from MODIS, GEOS-CHEM, CMAQ-AQS fusion model, and land use variables |
| Liu<br>(Bi et. al)                                     | PM <sub>2.5</sub>                                    | 1 x 1 km <sup>2</sup>   | NYS              | 2002-2016         | AOD from MODIS, gap filled with random forest approach, incorporating AQS data, land use regression variables, and meteorology from NARR        |
| OMI                                                    | NO <sub>2</sub>                                      | 0.1° x 0.1°             | Global           | 2005-2020         | OMI Version 4 NO <sub>2</sub> Surface Estimate                                                                                                  |
| WRF-CMAQ with AOD, CO                                  | NO <sub>2</sub> , PM <sub>2.5</sub> , O <sub>3</sub> | 12 x 12 km <sup>2</sup> | Global           | 2005-2020         | Reanalysis assimilating AOD retrievals from MODIS and CO retrievals from MOPITT into CMAQ, with WRF providing meteorological input              |



# bneR - workflow and collaborative modelling environment





# BNE workflow - configuration file

```
1 #-----#
2 #-----BNER CONFIGURATION FILE-----#
3 #-----#
4
5 ## preproc processes options
6 run_sp_context: TRUE # if TRUE spatial context will be intersected with inp
7 run_create_ref_grid: TRUE
8 run_keys_aqs : TRUE
9 run_keys_preds : TRUE
10 run_make_training_dta : TRUE
11 run_make_preds_dta : TRUE
12 ## bne processes options
13 run_bne_grid_search: FALSE
14 run_bne_cv: FALSE
15 run_bne_predict: FALSE
16 run_postprocess: FALSE
17
18
19 ### set input parameters
20 exp_folder_path : "/data0/shr/bne/exp/"
21 data_path : "/data0/shr/bne/data/"
22 ## general
23 expid : "exp_0068"
24 temp_resolution : "daily"
25 pollutant : "nox"
26 sp_context : "nys"
27 temp_context : 2015 # entire year that will be used for
28 input_base_model_names : ["cams","equates","js", "omi"]
29 obs_dta_name : "aqs"
30 # defining grids
31 ref_grid_from_input_base_model : 3 # write number referring
   this type of reference grid
32 ref_grid_resolution : NULL # in degrees (numeric); write
```

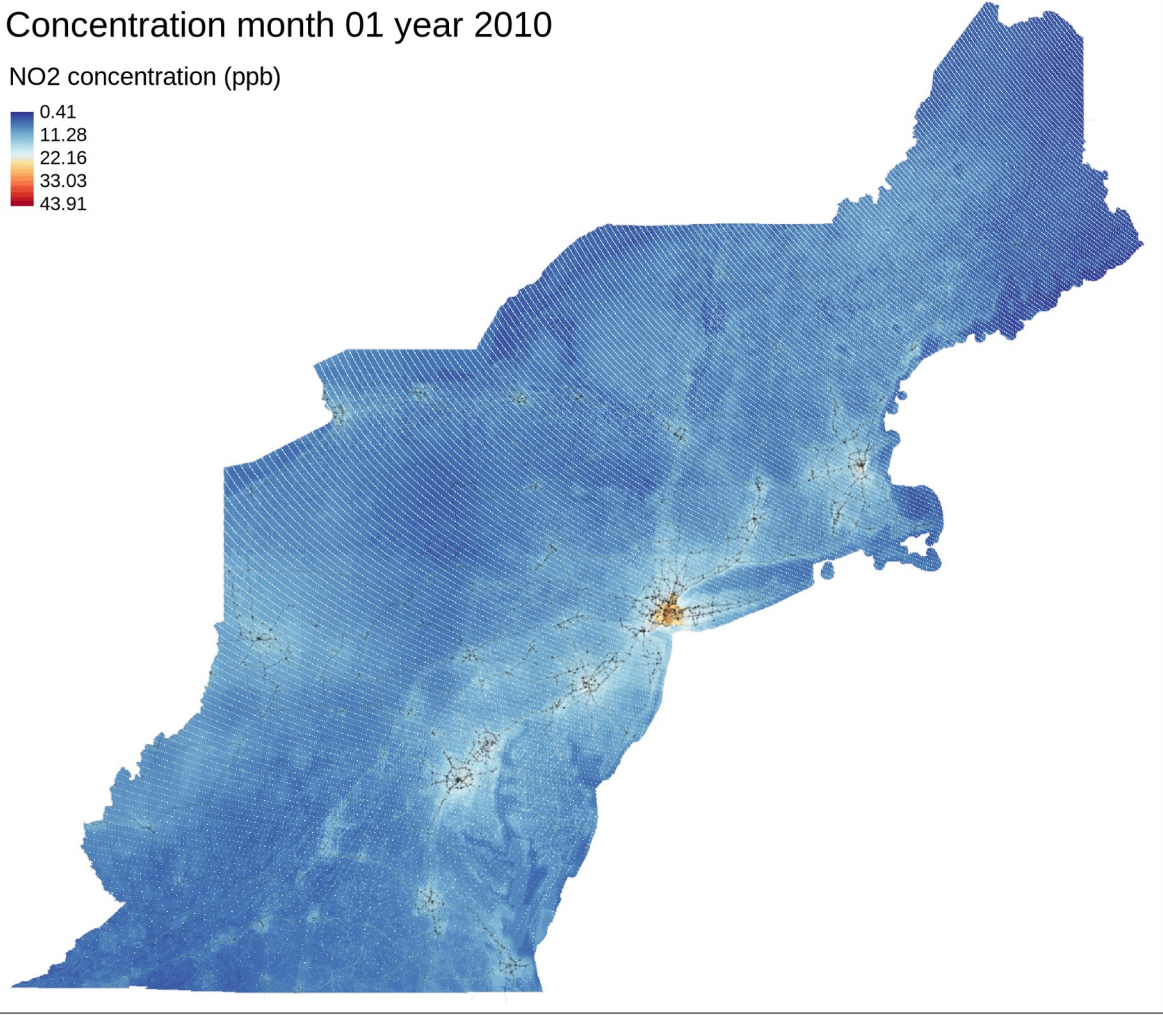
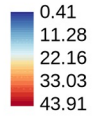
```
37 ### BNE run configuration
38 ## set parameters
39 time_var : 'percentOfYear'
40 # grid search (required to set the same number of
41 scale_space_w_list : [2, 1, 0.5] # [a, b, c] from a
42 scale_time_w_list : [2, 1, 0.5] # [a, b, c] from a
43 scale_space_rp_list : [2, 1, 0.5] # [a, b, c] from
44 scale_time_rp_list : [2,1,0.5] # [a, b, c] from a t
45 scale_space_wvar_list : [2,1,0.5] # [a, b, c] from
46 lambda_list : [0.3679, 0.1353, 0.0498, 0.0183] # s
47 lambda_rp_list : [0.3679, 0.1353, 0.0498, 0.0183]
48 seed_list : [1234] # set one seed
49 n_sample_list : [1000,2000] # set two n samples
50 # cross-validation
```

# Average concentrations

BNE: ["cams","equates","js"]

Concentration month 01 year 2010

NO2 concentration (ppb)

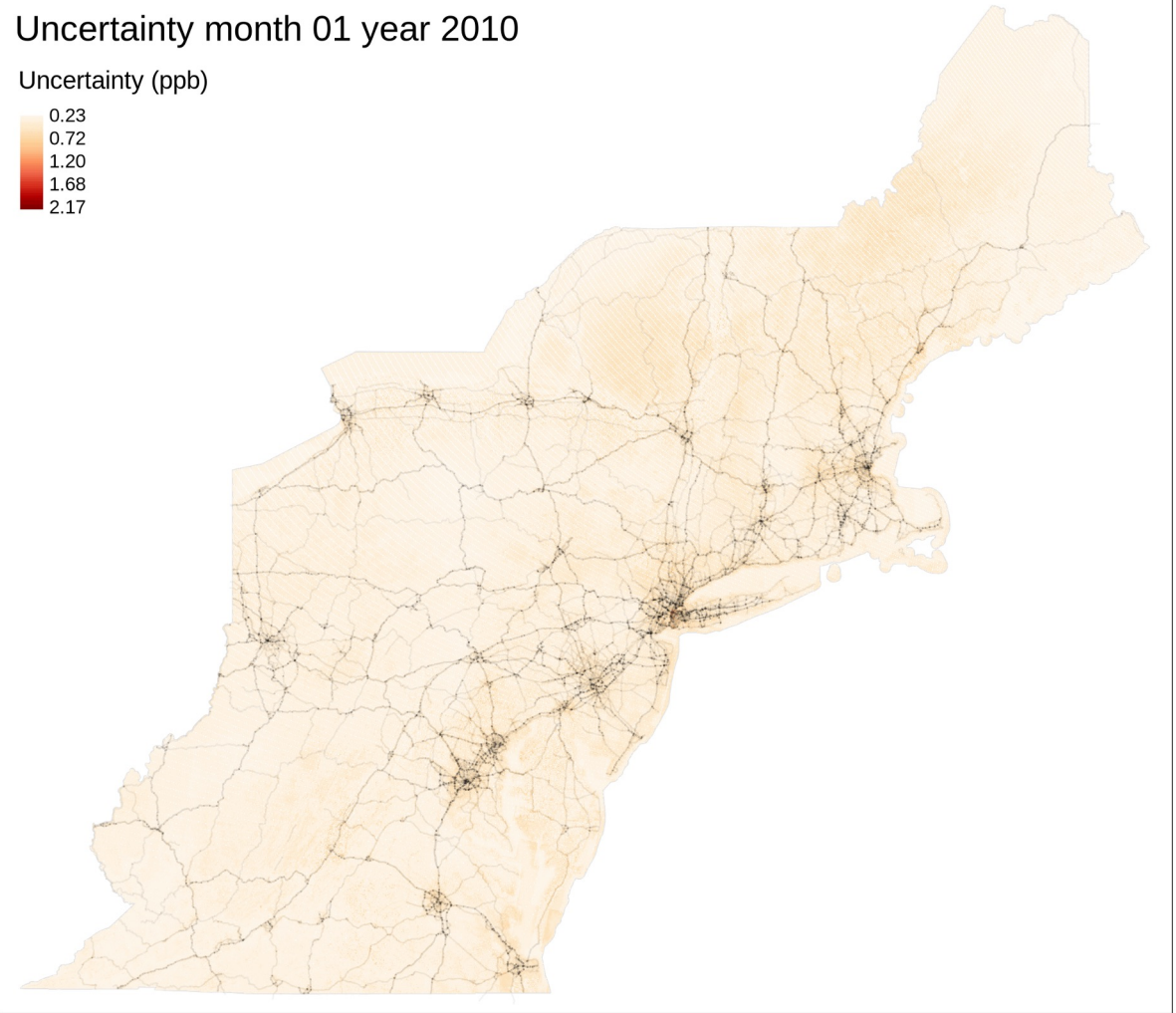
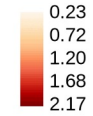


# Uncertainty

BNE: ["cams","equates","js"]

Uncertainty month 01 year 2010

Uncertainty (ppb)

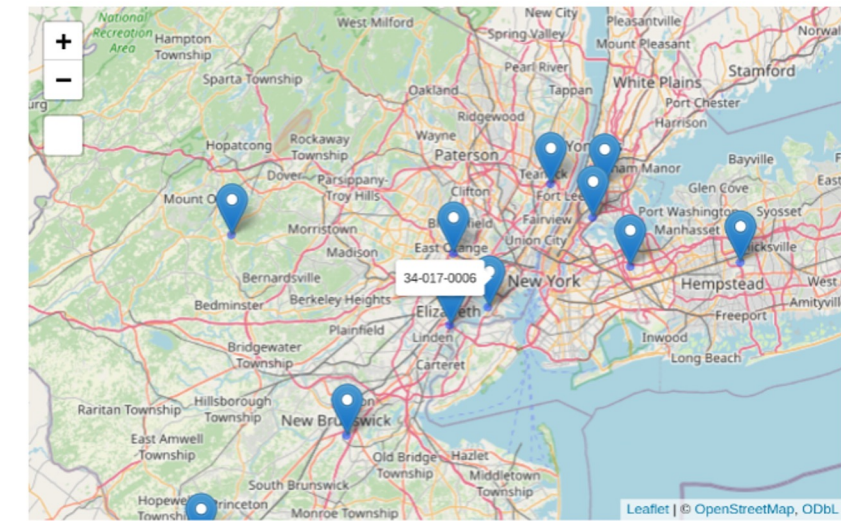


For preliminary results, please visit  
Vijay's Kumar poster on BNE!



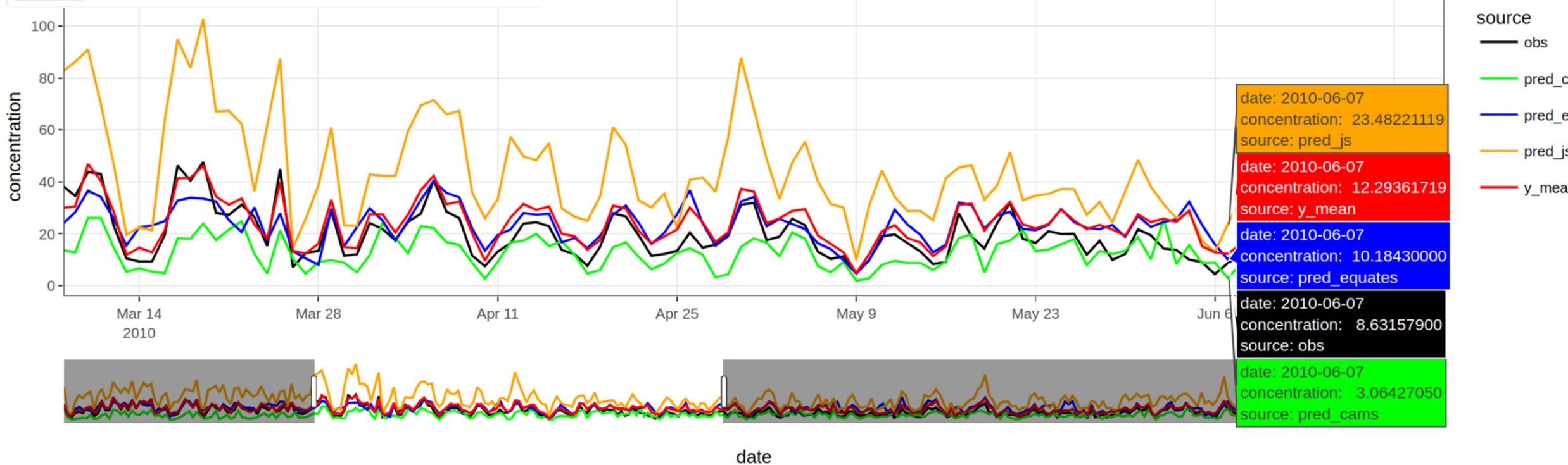


# Interactive exploration of results



AQS monitoring sites

34-017-0006

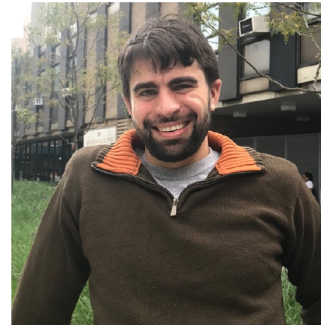




## Next: Co-producing data visualization for air pollutant concentration and uncertainty estimates

- **Objective:** Generate and disseminate data visualizations accounting for the needs of end-users and the integration of diverse expertises
- **Method:** Co-design of interactive visualizations to disseminate air pollutant concentrations and uncertainty estimates produced by BNE
- **Where:** Two online meetings to co-design and refine the co-developed interactive visualizations
- **When:** End of June ;)
- **Who:** Small group of potential users (e.g., health studies, policy making, etc..). **If interested, please let us know**

## BNE team



Thank you!!  
Jaime Benavides  
[jap2312@cumc.columbia.edu](mailto:jap2312@cumc.columbia.edu)