A Data Fusion Approach for Space-Time Analysis of Speciated $PM_{2.5}$

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Background

Fine particulate matter ($PM_{2.5}$) is an EPA regulated air pollutant linked to a variety of adverse health effects

- Classified based on particle size (< 2.5 μm diameter)
- Major species: Sulfate, Nitrate, Ammonium, Soil, Carbon.
- Minor species: trace elements (K, Mg, Ca), heavy metals (Cu, Fe), etc.
- Complex spatio-temporal dependence between species

Data (2007)

Speciated $PM_{2.5}$ Sources

- Chemical Speciation Network (CSN) - 221 stations
- Interagency Monitoring of Protected Visual Environments (IMPROVE) - 172 stations

Total $PM_{2.5}$ Sources

- Federal Reference Method (FRM) - 949 stations

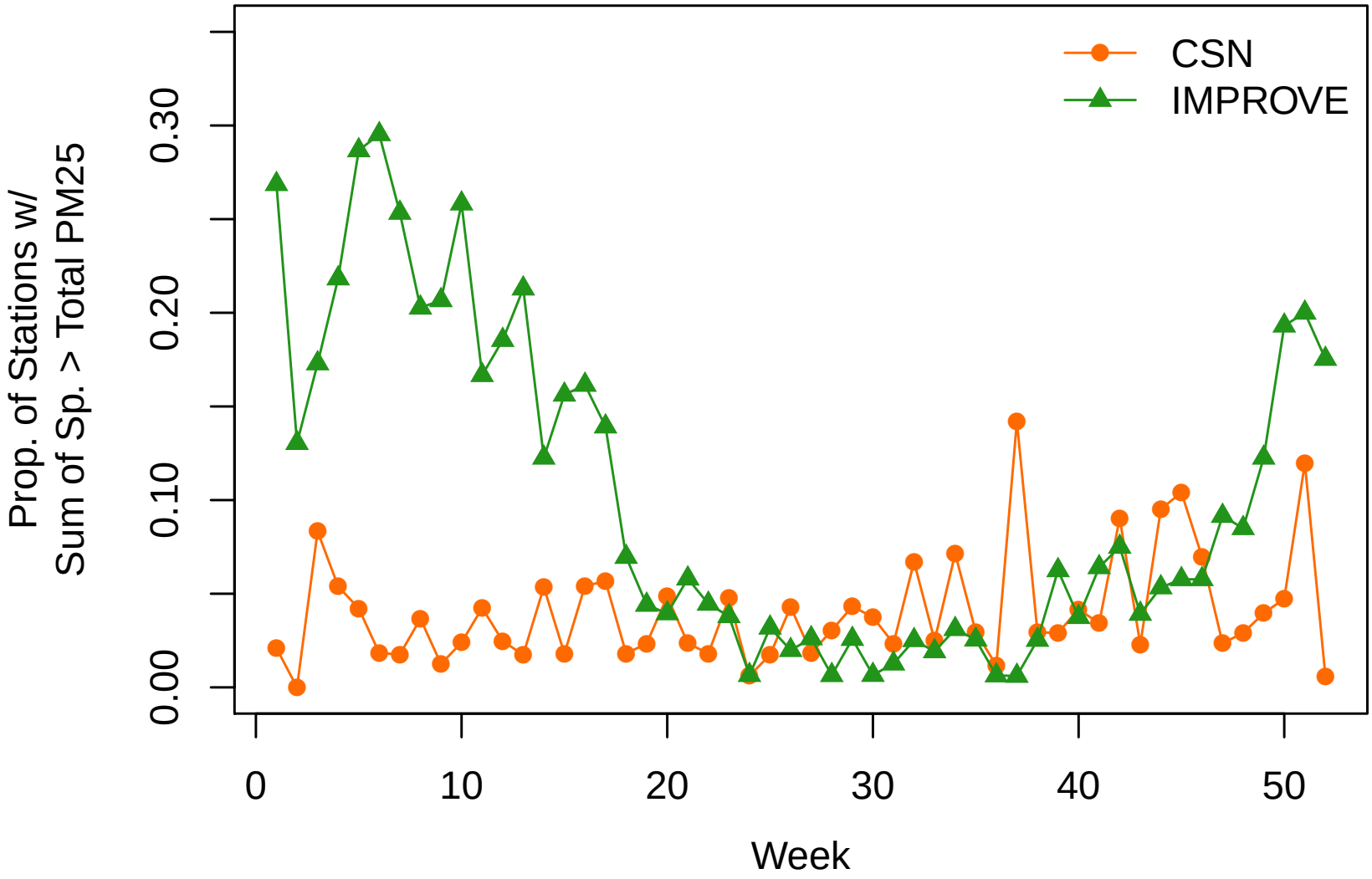
Model Output

- Community Multi-scale Air Quality (CMAQ) - 12 km grid

Data Issues

- Monitoring frequency
- Total vs Sum of Species

Total $PM_{2.5}$ vs Sum of Species



Species Model Details

For the 5 major species (Sulfate, Nitrate, Ammonium, Soil, Carbon) and the two networks (CSN, IMPROVE):

$$C_t^i(\boldsymbol{s}) = Z_t^i(\boldsymbol{s}) + \epsilon_{C,t}^i(\boldsymbol{s})$$
$$I_t^i(\boldsymbol{s}) = Z_t^i(\boldsymbol{s}) + \epsilon_{I,t}^i(\boldsymbol{s})$$

where $Z_t^i(\boldsymbol{s})$ are the latent "true" concentrations of species i at time t and locations $\boldsymbol{s}$,

$$Z_t^i(\boldsymbol{s}) = \max\left(0,\ \widetilde{Z}_t^i(\boldsymbol{s})\right)$$
$$\widetilde{Z}_t^i(\boldsymbol{s}) = \beta_{0,t}^i + \beta_{0,t}^i(\boldsymbol{s}) + \beta_{1,t}^i\, Q_t^i(B_{\boldsymbol{s}})$$

Total $PM_{2.5}$ Model Details

For total $PM_{2.5}$ from the three networks (CSN, IMPROVE, FRM):

$$C_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{C,t}^{tot}(\boldsymbol{s})$$
$$I_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{I,t}^{tot}(\boldsymbol{s})$$
$$F_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{F,t}^{tot}(\boldsymbol{s})$$

where $Z_t^{tot}(\boldsymbol{s})$ are the latent "true" concentration of total $PM_{2.5}$ at time t and locations $\boldsymbol{s}$, which is given by the sum of the major species and the "other" species concentrations.

$$Z_t^{tot}(\boldsymbol{s}) = \sum_{i=1}^{5} Z_t^i(\boldsymbol{s}) + Z_t^o(\boldsymbol{s})$$

$$Z_t^o(s) = \max\left(0,\ \widetilde{Z}_t^o(s)\right) \qquad \widetilde{Z}_t^o(\boldsymbol{s}) = \beta_{0,t}^o + \beta_{0,t}^o(\boldsymbol{s}) + \beta_{1,t}^o\, Q_t^o(B_{\boldsymbol{s}})$$

Spatial Dependence

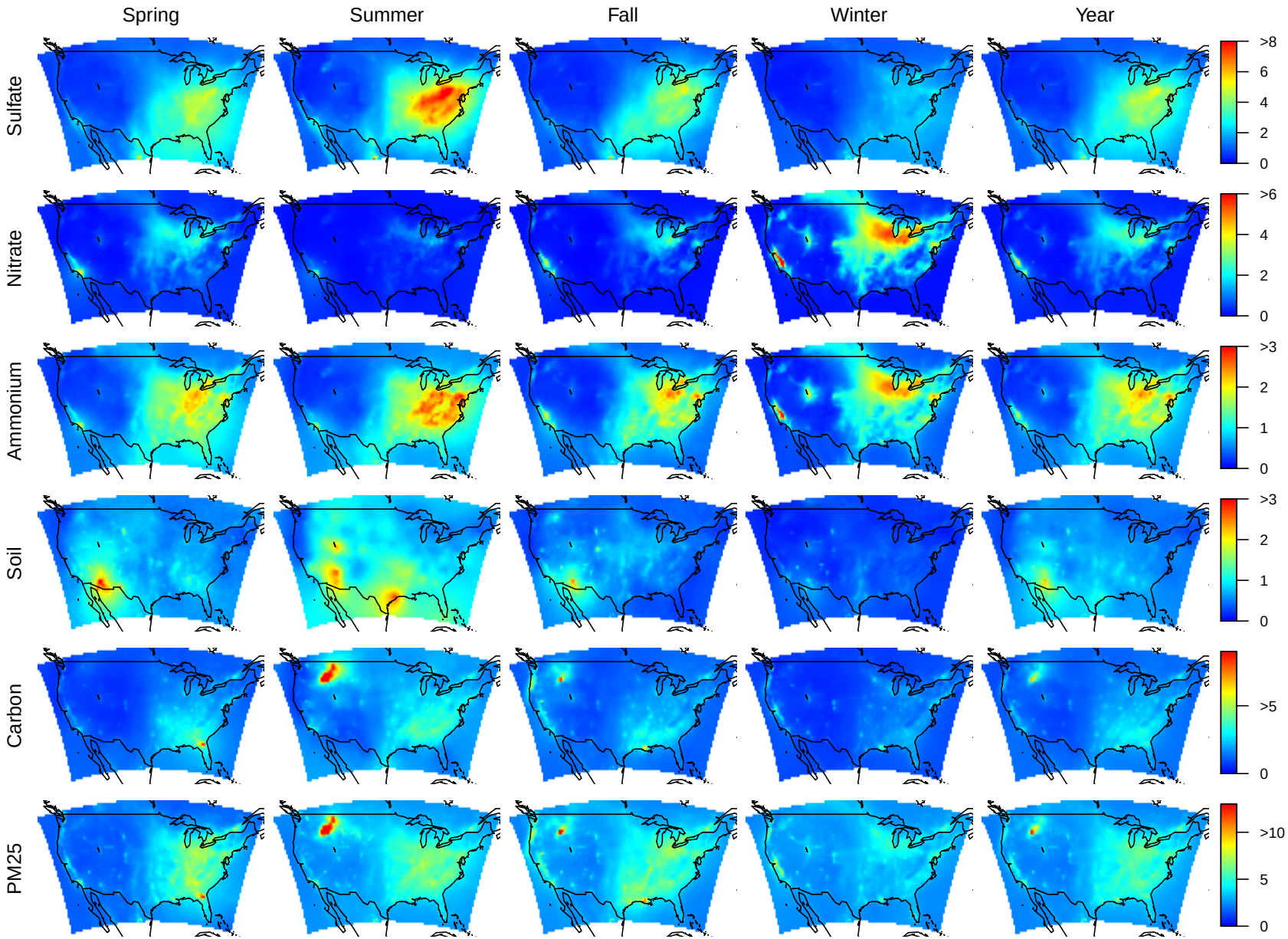
Spatial dependence enters the model through the $\beta^i_{0,t}(s)$ parameters for $i \in \{o, 1, 2, 3, 4, 5\}$.

$$\beta^i_{0,t}(\boldsymbol{s}) = \sigma^i_t \; w^i_t(\boldsymbol{s})$$

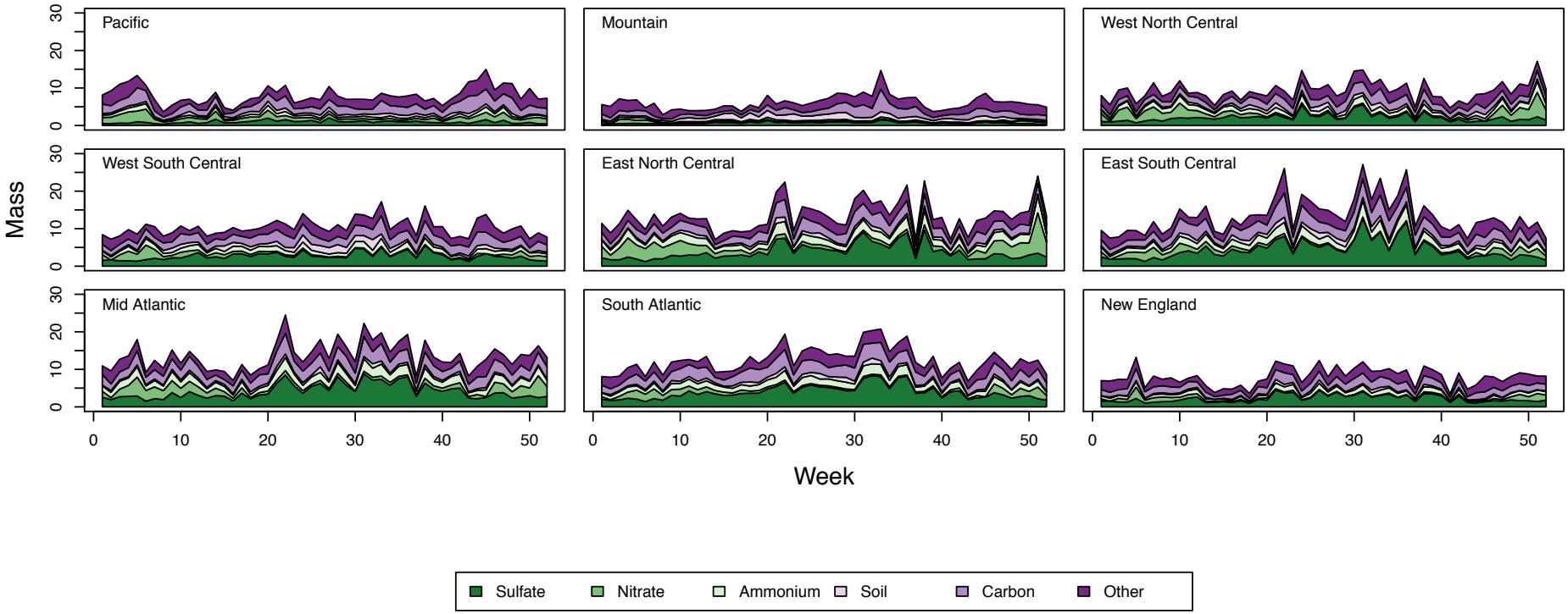
where $w^i_t(\boldsymbol{s})$ are zero mean, variance 1, Gaussian processes with exponential correlation given by

$$\text{corr}(w^i_t(\boldsymbol{s}), w^i_t(\boldsymbol{s}')) = \exp(-\phi^i_t|\boldsymbol{s} - \boldsymbol{s}'|)$$

Model results



Model results



Model Validation

		Sulfate	Nitrate	Ammonium	Soil	Carbon	PM25
RMSE	Tobit w/o CMAQ	1.347	2.257	0.858	1.363	3.073	6.298
	Tobit	1.151	1.641	0.724	1.307	2.851	5.393
CRPS	Tobit w/o CMAQ	0.639	0.758	0.374	0.468	1.064	3.023
	Tobit	0.554	0.558	0.329	0.438	0.885	2.452
EmpCov	Tobit w/o CMAQ	0.935	0.931	0.933	0.907	0.923	0.924
	Tobit	0.920	0.930	0.924	0.915	0.921	0.906

Validation based on randomly selecting 10% of stations as hold outs.

Run times

Total run time for model fitting (50,000 iterations):

- CPU - 7.7 hours
- CPU+GPU - 4.8 hours

$\times$ 52 weeks

Total run time for model prediction at 5950 locations (1,000 iterations):

- CPU - 7.2 hours
- CPU+GPU - 4.3 hours

$\times$ 52 weeks

One run takes about 775 hours total on CPU alone, 473 on CPU and GPU.

Model fitting performance

Parameter	CPU (secs)	CPU+GPU (secs)	Rel. Performance
$\beta_0,\ \beta_1$	0.00029	0.00030	0.97
$\beta_0(s)$	0.09205	0.09132	1.00
σ	0.00383	0.00385	0.99
ϕ	0.46084	0.25174	1.83
ϵ	0.00003	0.00003	1.00
Total	0.55708	0.34729	1.60

Acknowledgments

- Alan Gelfand - Duke
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- Erin Schliep - Duke
- Wyat Apel - NERL

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Information & Questions

Email : rundel@gmail.com

Presentation : `http://github.com/rundel/Presentations/`

Paper : Rundel C., Schliep E., Holland D., Gelfand A. (2014) A data fusion approach for space-time analysis of speciated PM2.5. *The Annals of Applied Statistics*. *In submission*

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Questions?

Performance

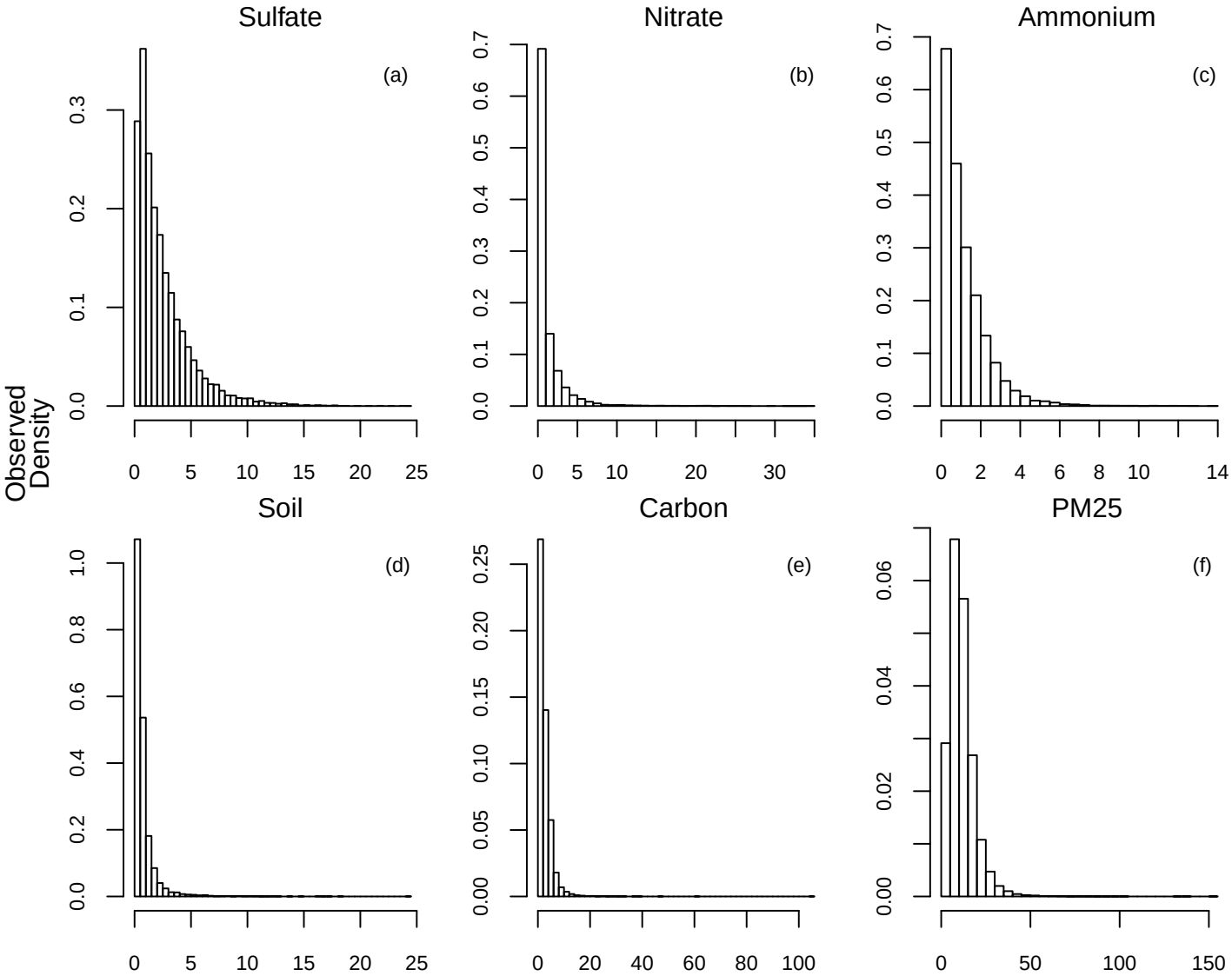
System Specs:

- 4 core Intel i5-2500K @ 3.30 GHz
- 16 GB DDR3 @ 1333 MHz
- GeForce GTX 460

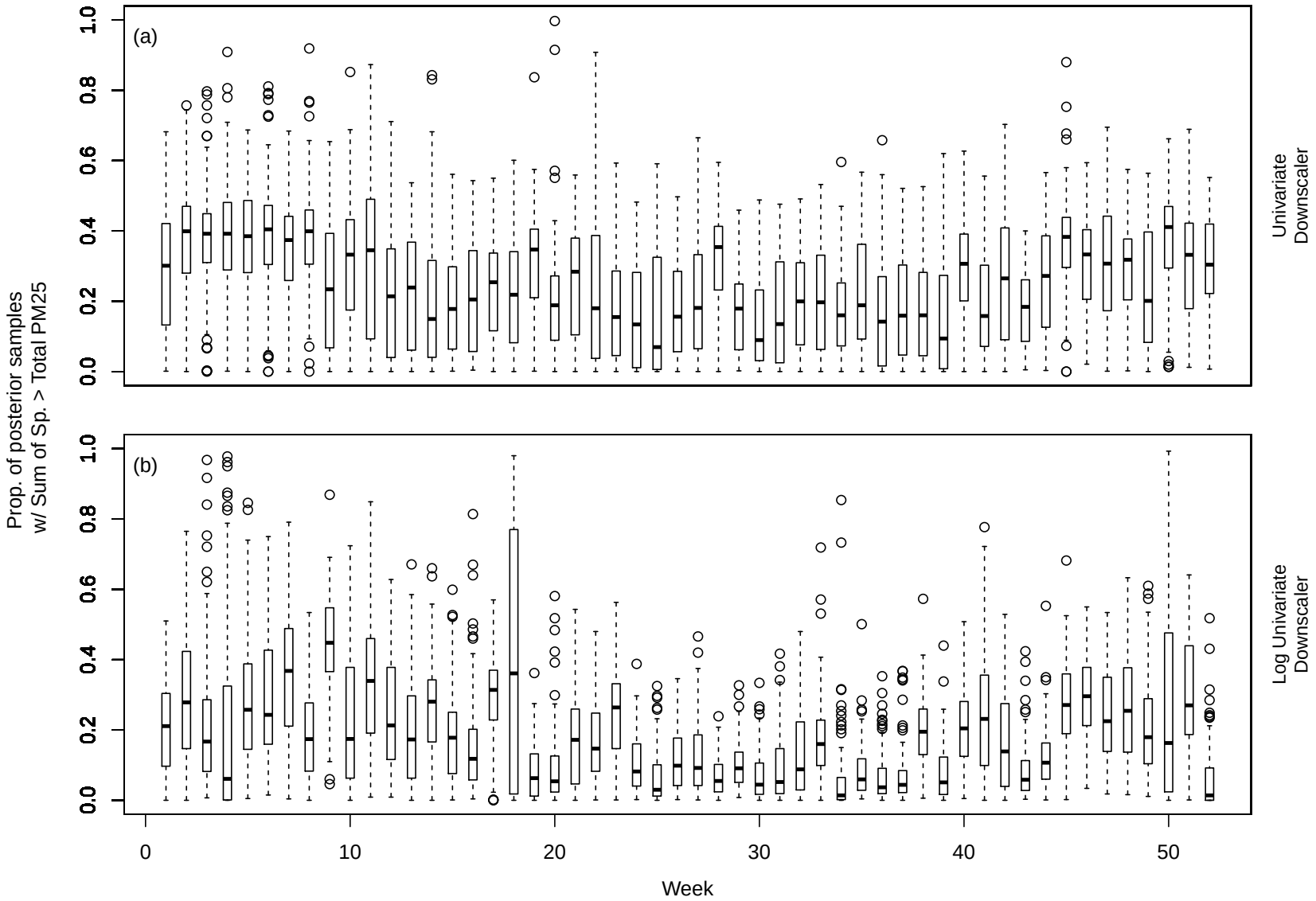
Software Specs:

- Ubuntu 13.10
- OpenBlas 0.2.8
- CUDA 6.0RC
- Magma 1.4.1

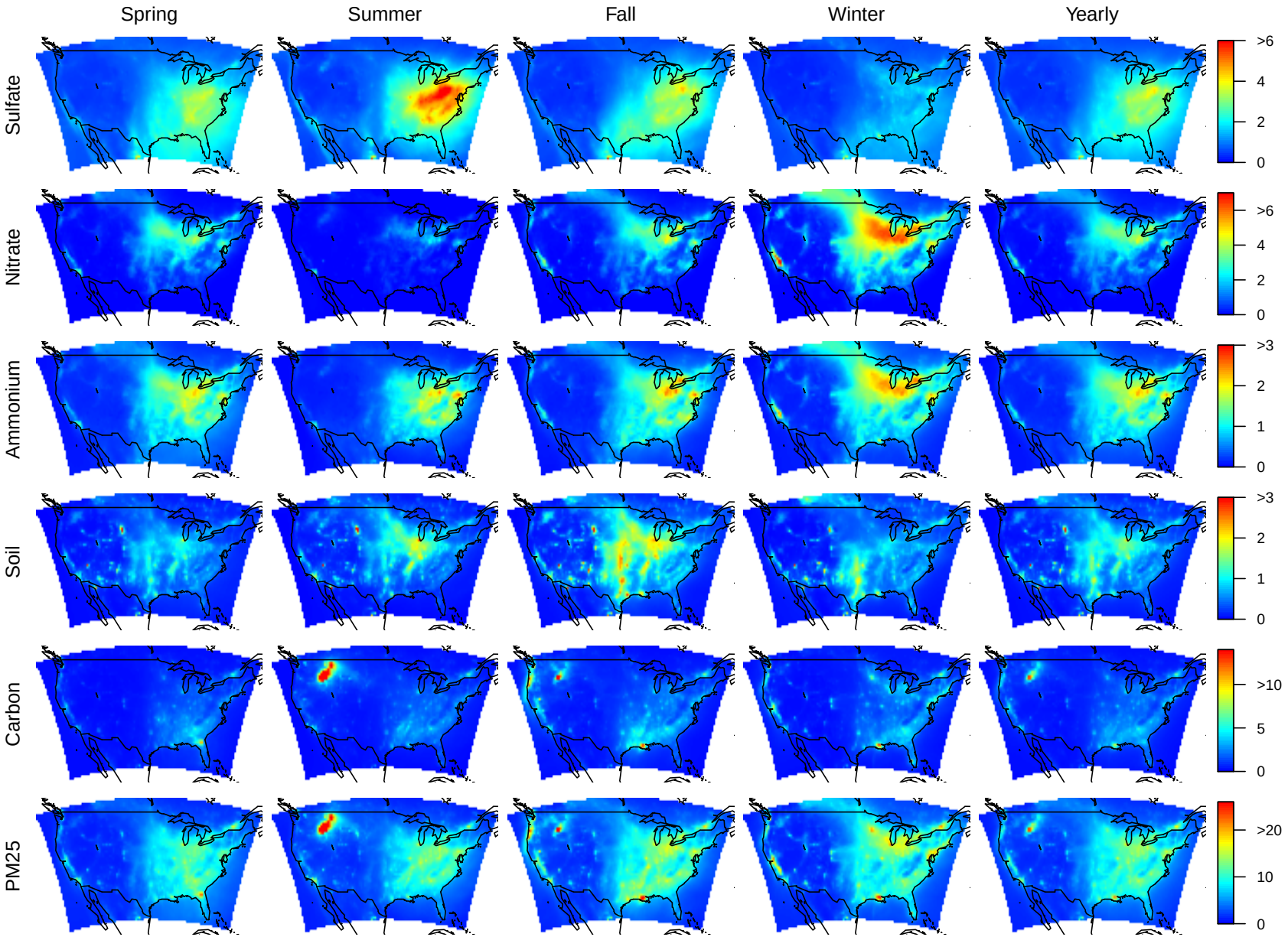
Species Distributions



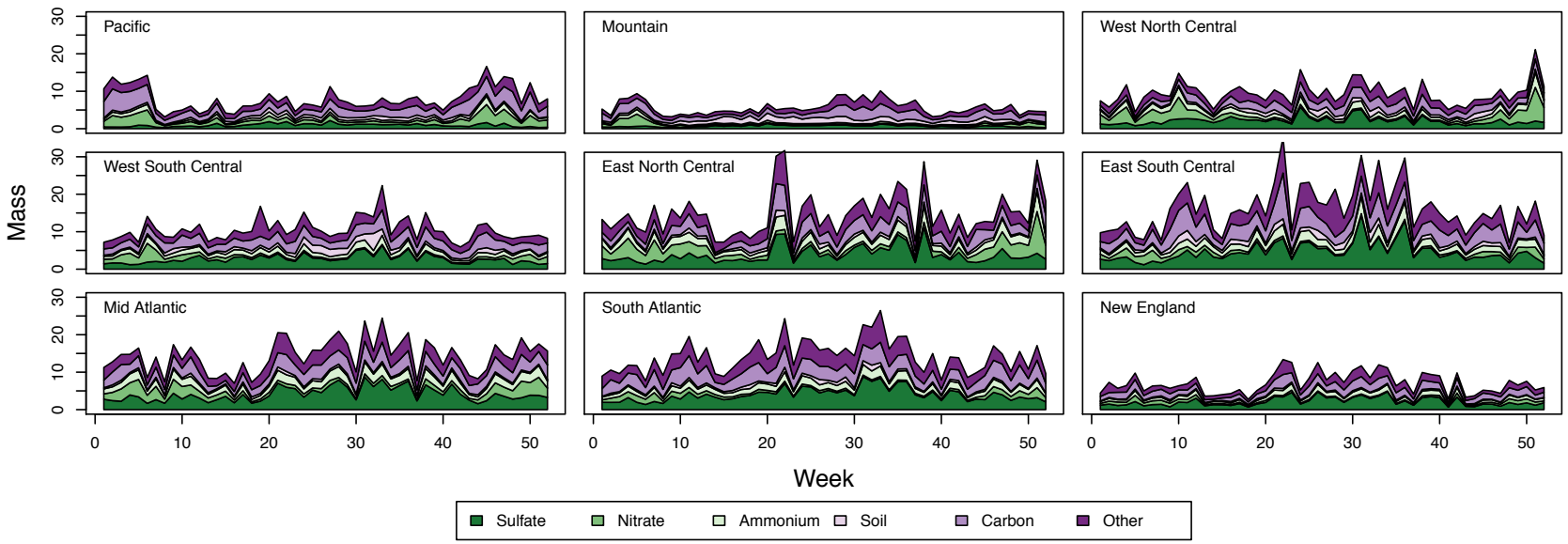
Univariate Model Exceedance



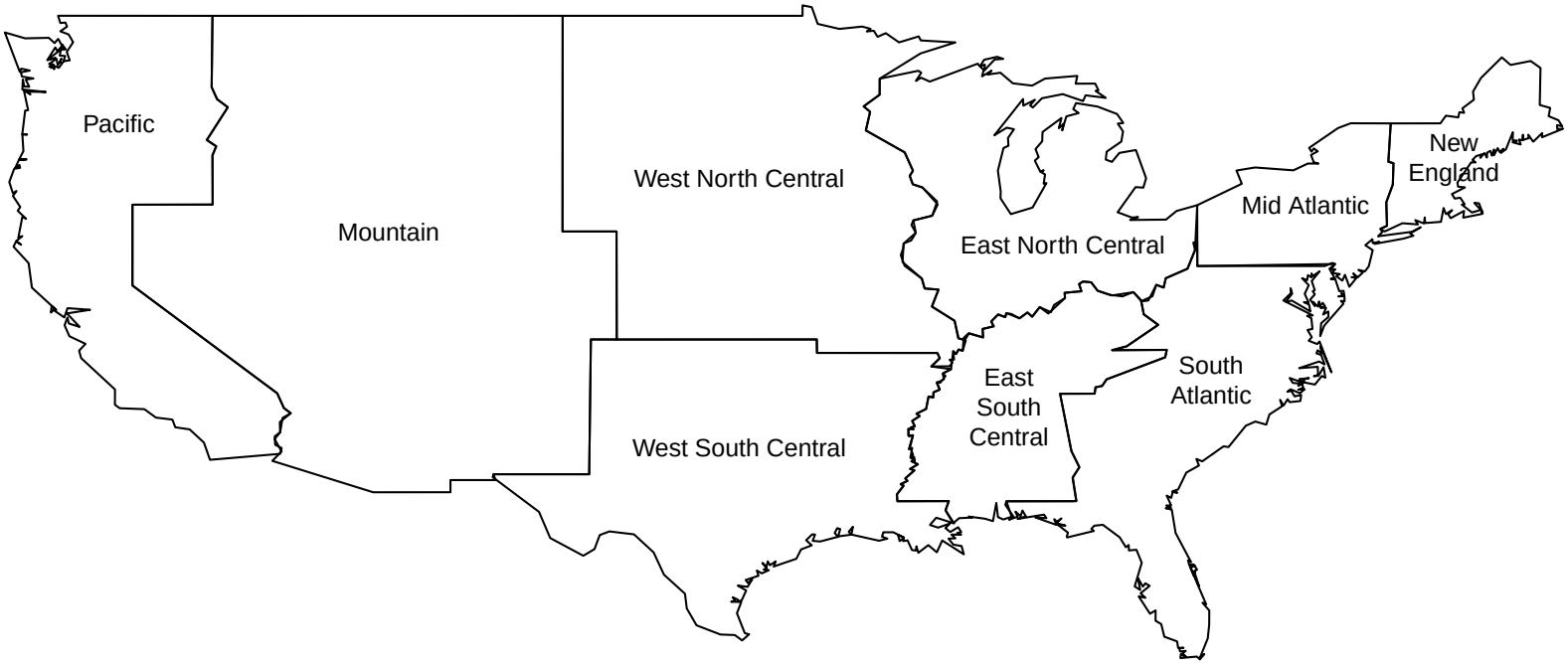
CMAQ Maps


Spring
Summer
Fall
Winter
Yearly
Sulfate
Nitrate
Ammonium
Soil
Carbon
PM25
>6
4
2
0
>6
4
2
0
>3
2
1
0
>3
2
1
0
>10
5
0
>20
10
0

Data TS


Pacific
Mountain
West North Central
West South Central
East North Central
East South Central
Mid Atlantic
South Atlantic
New England
Mass
Week
0
10
20
30
40
50
Sulfate
Nitrate
Ammonium
Soil
Carbon
Other

Regions


Pacific
Mountain
West North Central
East North Central
Mid Atlantic
New England
West South Central
East South Central
South Atlantic