Source Estimation and Atmospheric Modelling: Uncertainties Quantification

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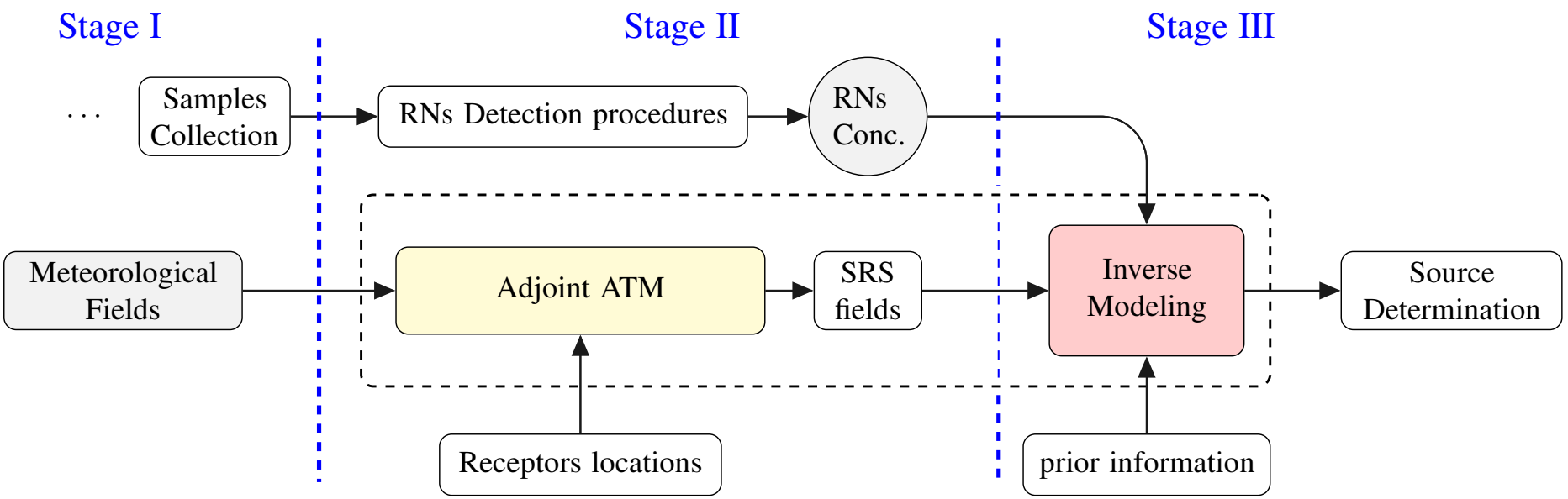
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Source Determination By Using ATM



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Sources of Uncertainties in Source Determination

- Atmospheric Fields Uncertainties:
  - Instrumental Errors of Meteorological observations.
  - representativeness Errors.
  - Modeling Errors
    - Approximation of Complex Atmosphere-Ocean-Land interactions.
    - Unresolved Atmospheric Scales. (Parameterization)
    - Turbulence (The last unsolved problem of classical physics.)
    - Sensitivity in initial and boundary conditions.
- Radionuclide concentrations Measurements:
  - Instrumental Accuracy.
  - Sampling (Misrepresentative Samples)
  - Uncertainties in radionuclides Analyses

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Facing Uncertainties

- Q: How can we deal with these uncertainties?

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- A1: Ensemble Techniques.

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Facing Uncertainties

- Q: How can we deal with these uncertainties?
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- A2: Bayesian Inference Approach

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Facing Uncertainties

- Q: How can we deal with these uncertainties?
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- Q: How can the uncertainty be quantified ?

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Facing Uncertainties

- Q: How can we deal with these uncertainties?
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- Q: How can the uncertainty be quantified ?
- A: The probability density function; PDF

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Time Evolution of Atmospheric Variables

Deterministic Model:

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Time Evolution of Atmospheric Variables

Deterministic Model:

$$T_{t_0}, U_{t_0} \xrightarrow{\text{time}} T_{t_1}, U_{t_1}$$

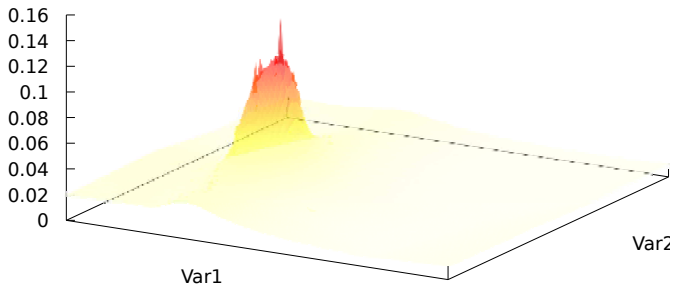
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Probabilistic Approach:



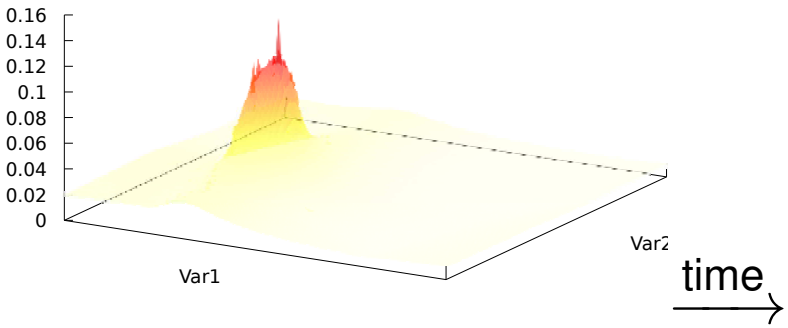
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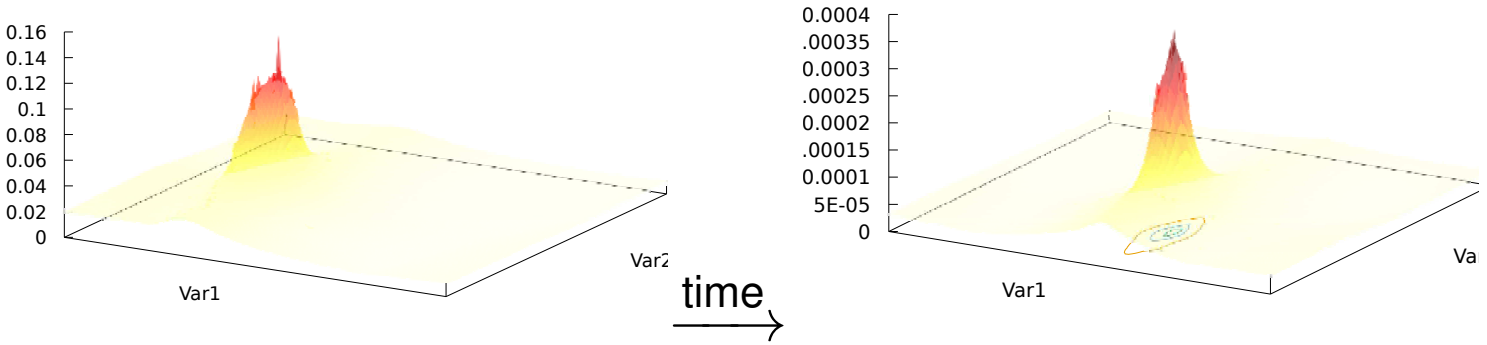
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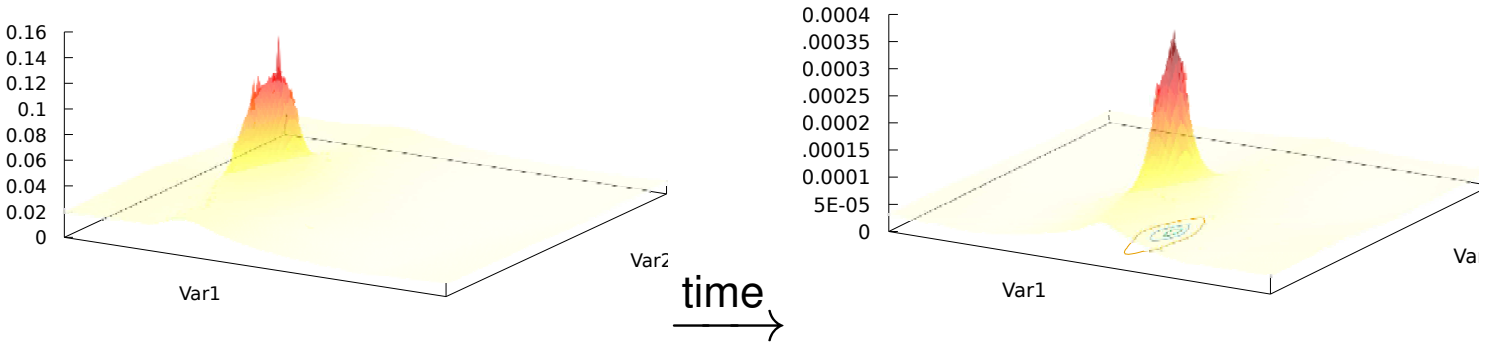
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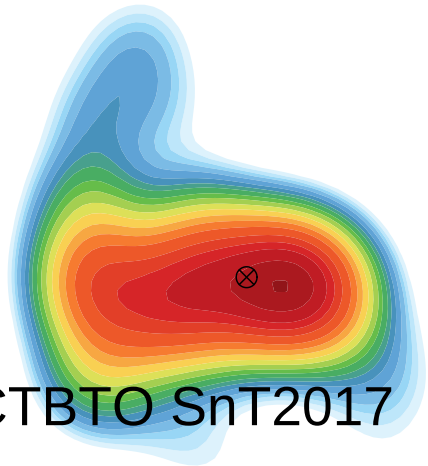
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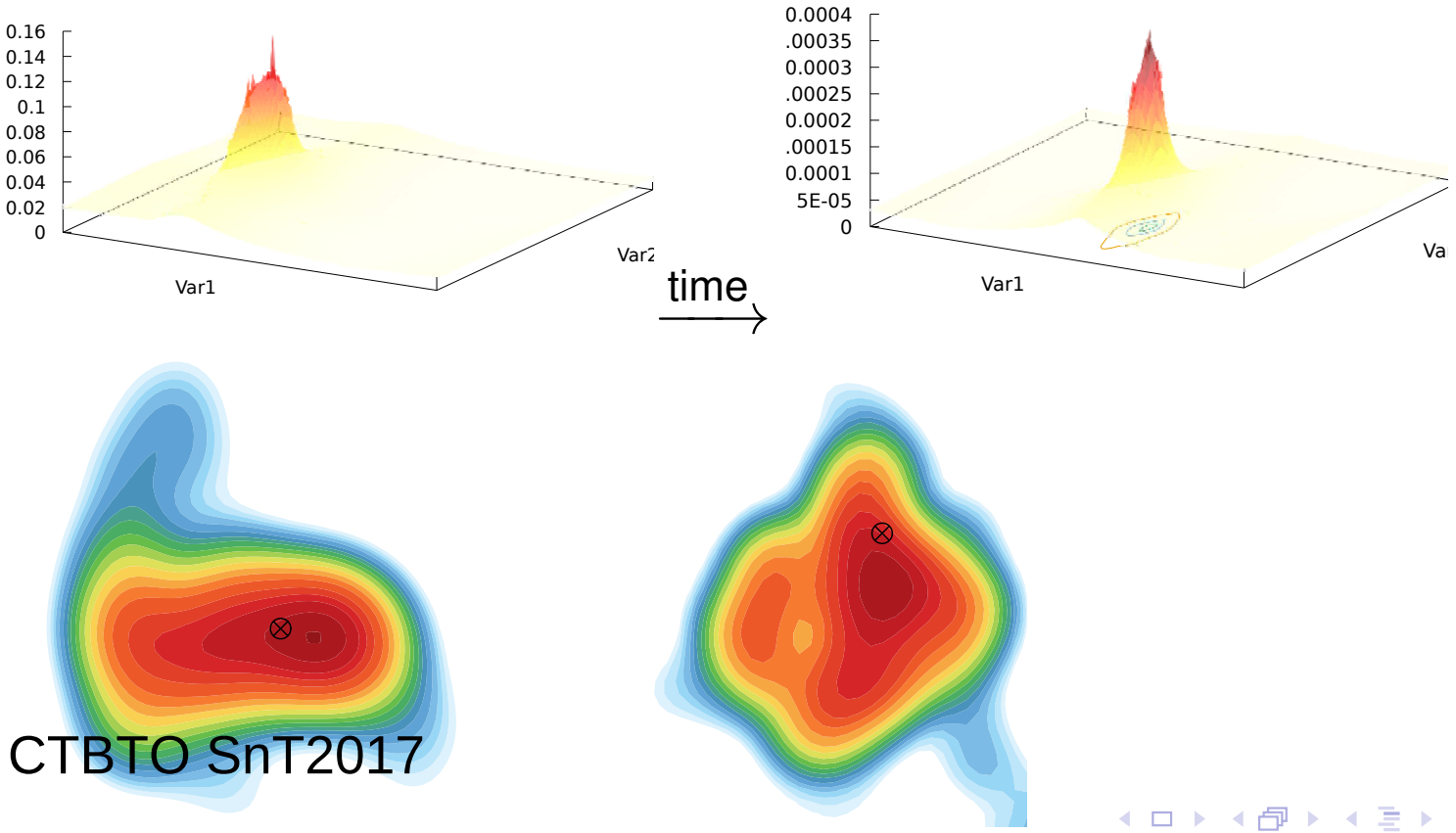
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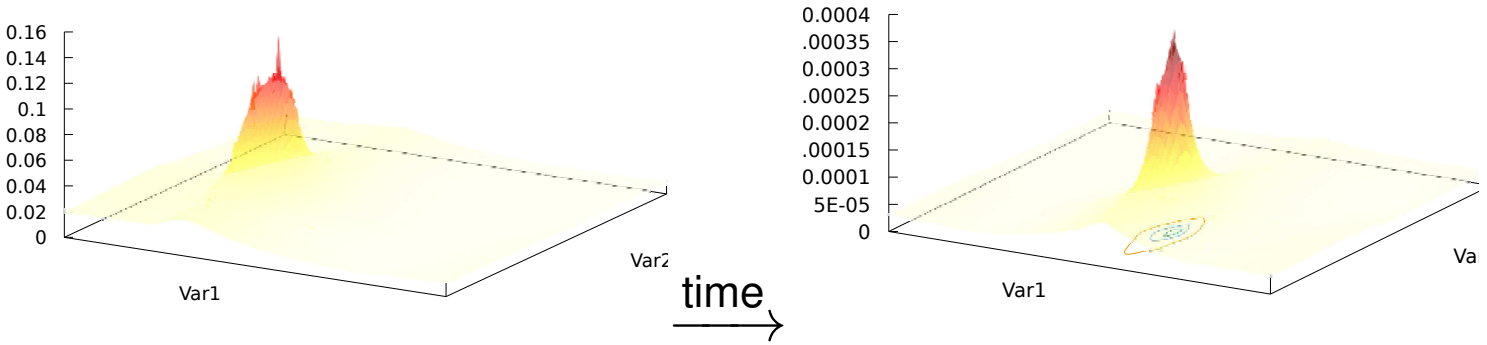


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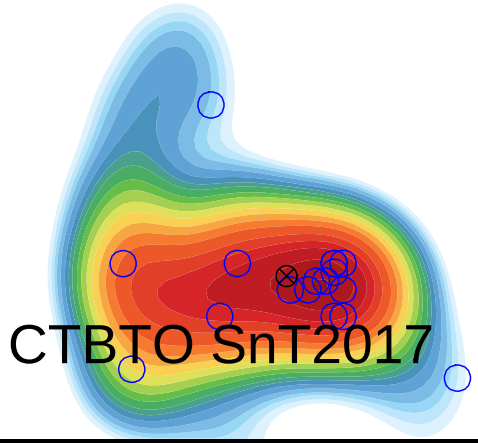
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Probabilistic Approach:



Ensemble Approach:

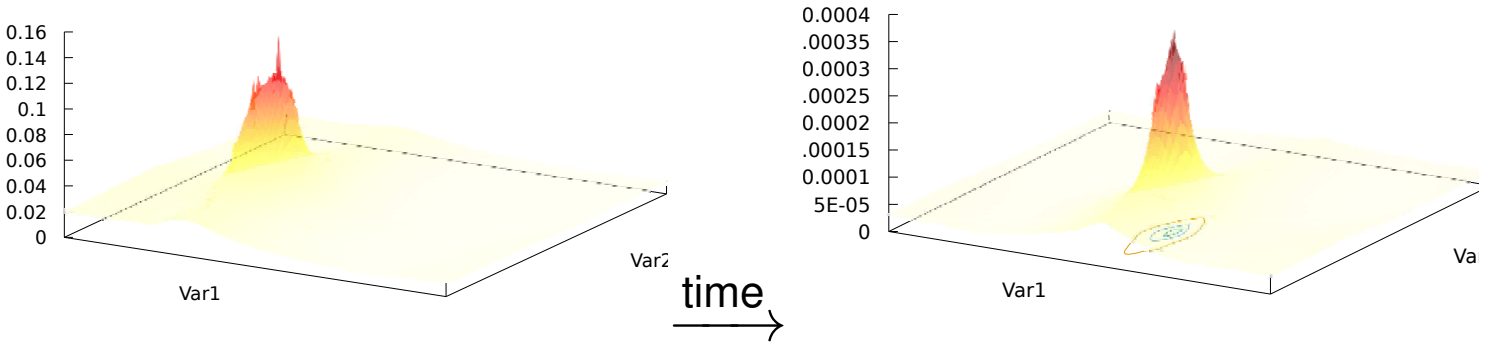


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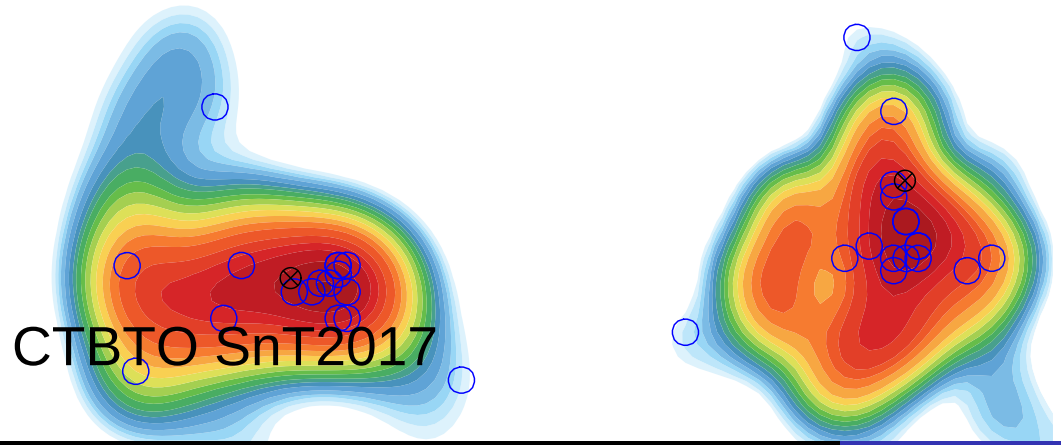
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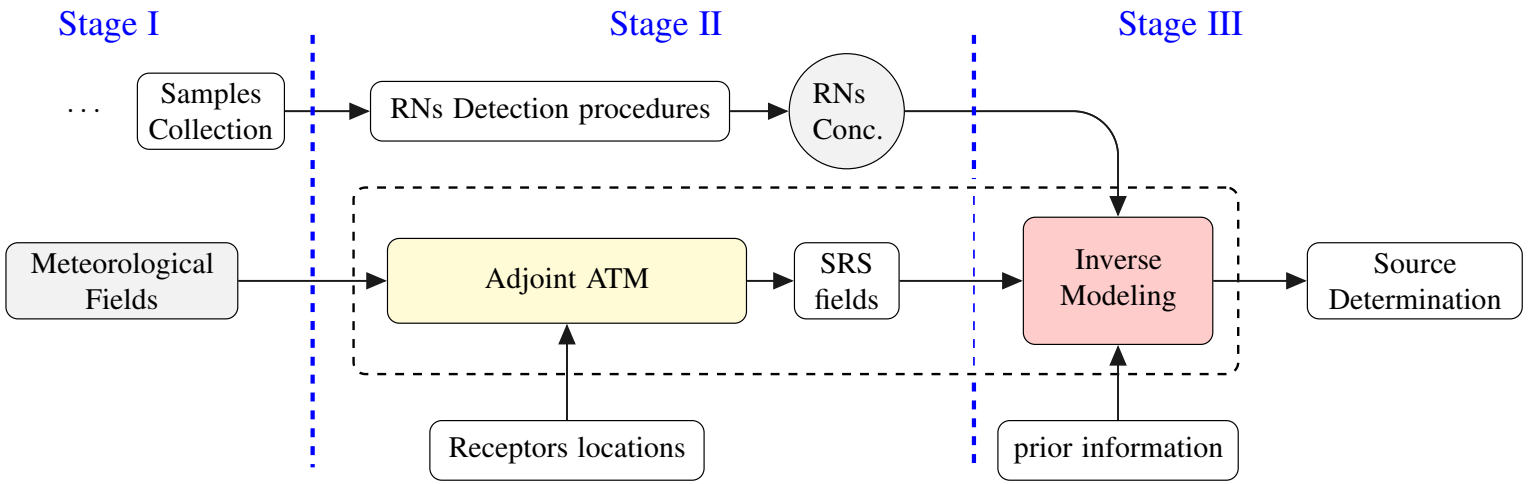
Ensemble Approach:



Configuration of Numerical Experiments

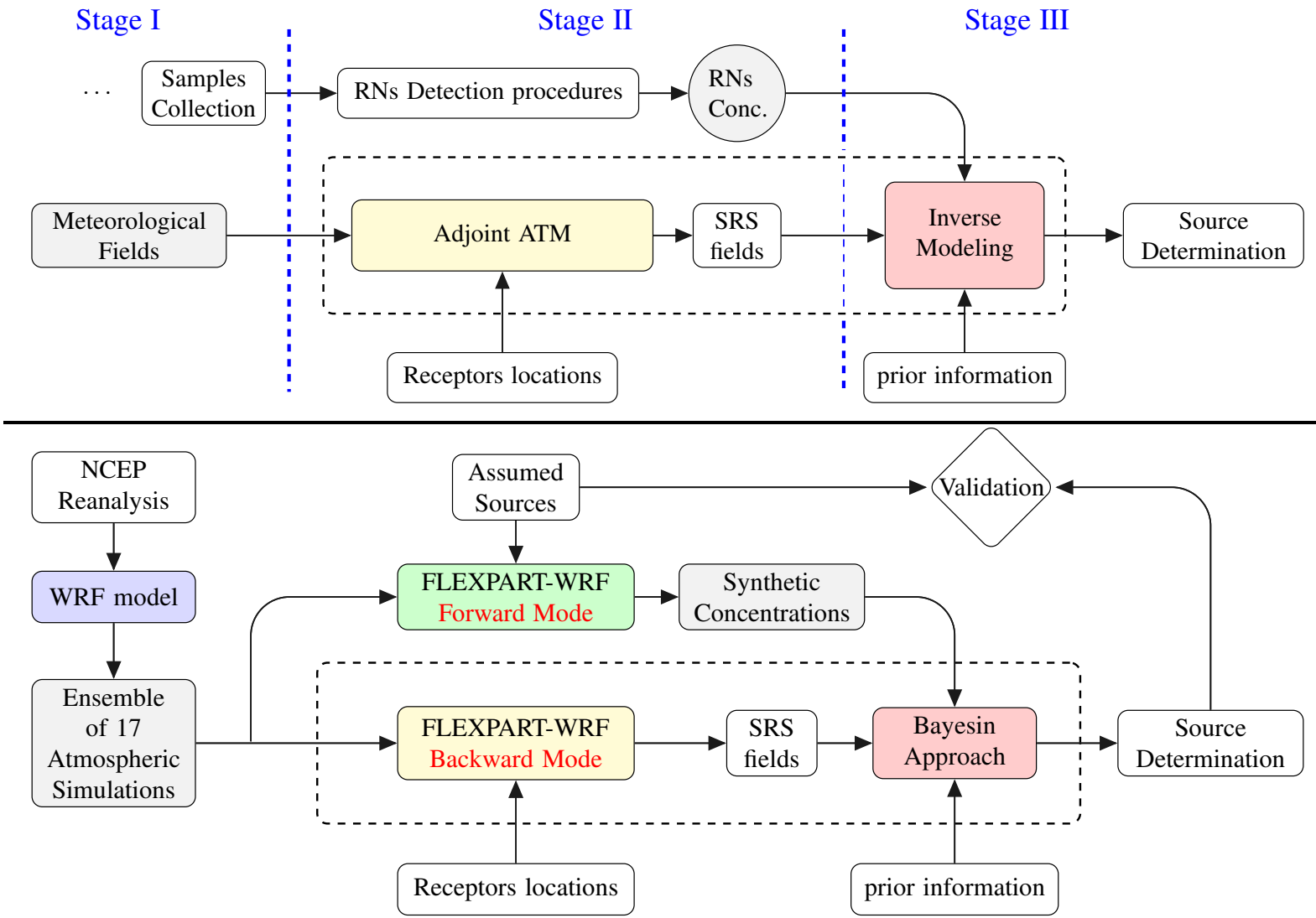
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Experimental Design



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Experimental Design



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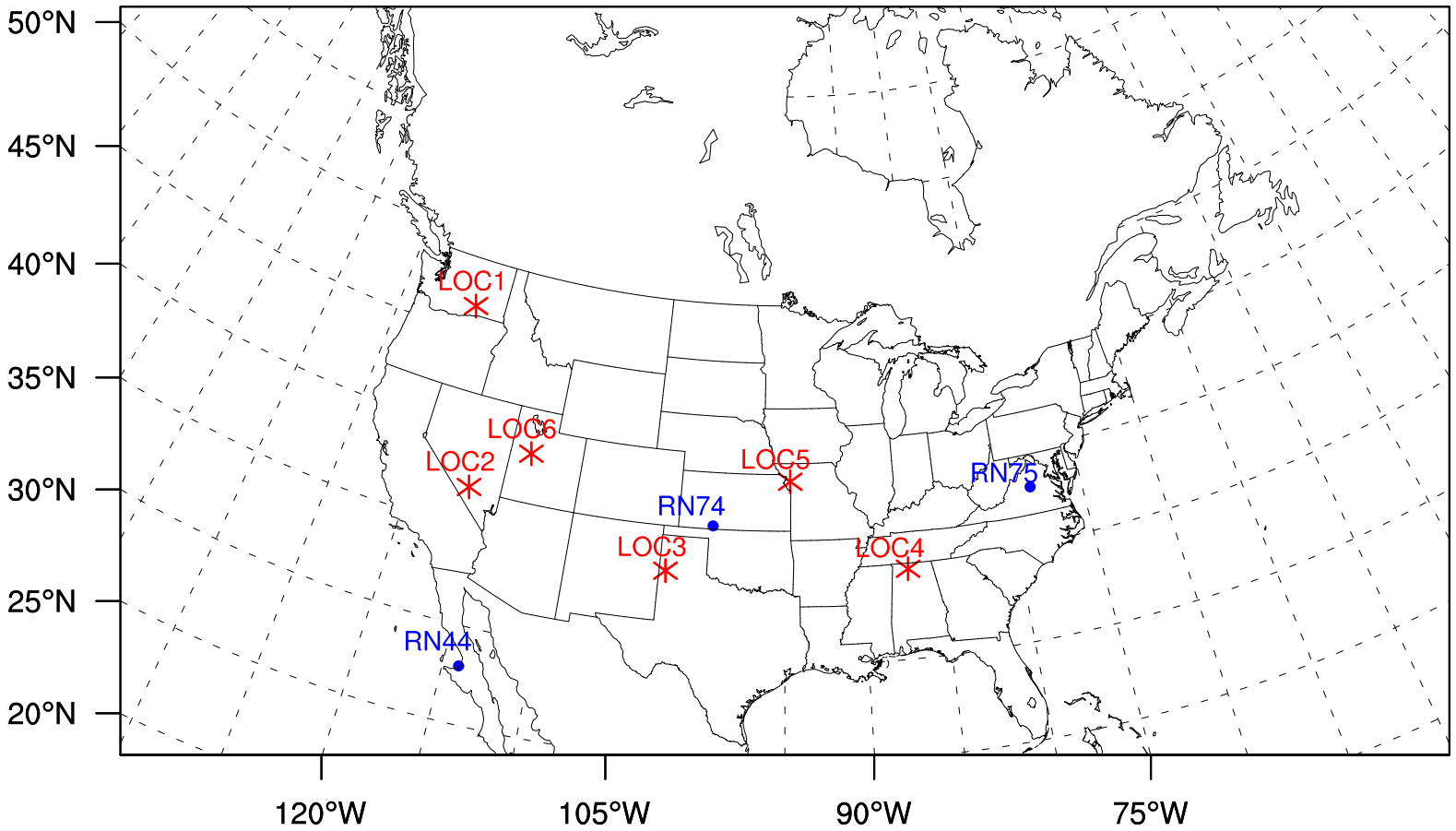
Numerical Experiement

- Atmospheric Simulation
  - Time Domain: 00 UTC on 6^{th}Oct.– 00 UTC 16^{th} Oct. 2014.

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Numerical Experiement

- Atmospheric Simulation
  - Time Domain: 00 UTC on 6^{th}Oct.– 00 UTC 16^{th} Oct. 2014.
  - Spatial Domain: Grid distance $\simeq 33km$.



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Numerical Experiement

- Atmospheric Simulation
  - Time Domain: 00 UTC on 6^{th}Oct.– 00 UTC 16^{th} Oct. 2014.
  - Spatial Domain: Grid distance $\simeq 33km$.
  - Initial and Boundary conditions: NCEP Reanalysis, (Grid distance $\simeq 1^{o}$).

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Numerical Experiement

- Atmospheric Simulation
  - Time Domain: 00 UTC on 6^{th}Oct.– 00 UTC 16^{th} Oct. 2014.
  - Spatial Domain: Grid distance $\simeq 33km$.
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  - WRF model (ARW v3.7) with 17 different configurations;

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Numerical Experiement

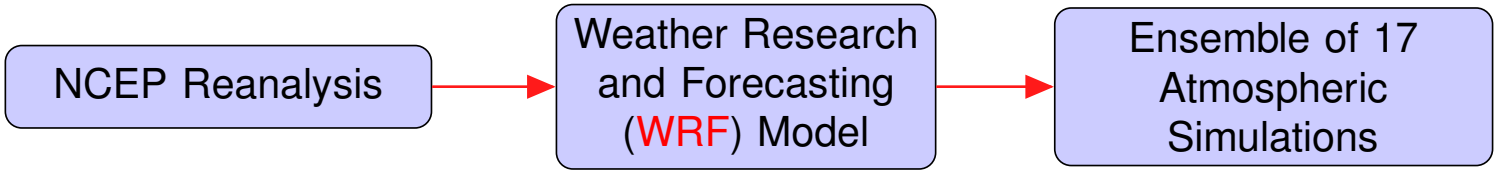
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  - WRF model (ARW v3.7) with 17 different configurations;

Ensemble Member	PBL Scheme	Micro–physics
1	MYNN2	WSM3
2	MYNN3	WSM3
3	ACM2	WSM3
4	Boulac	WSM3
5	Shin-Hong	WSM3
6	UW	WSM3
7	MRF	WSM3
8	YSU	WSM3
9	YSU	WSM5
10	YSU	WSM6
11	YSU	Kessler
12	YSU	Eta
13	YSU	Thompson
14	YSU	Morrison 2-mom
15	YSU	CAM 5.1
16	YSU	WDM6
17	YSU	NSSL 2-mom w/o hail

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Numerical Experiement

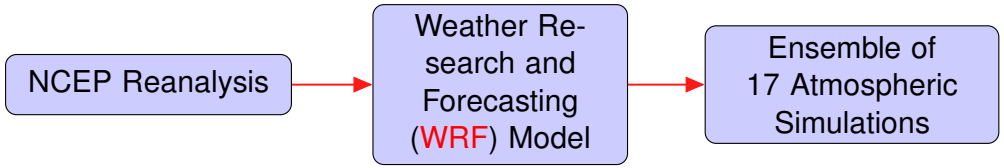
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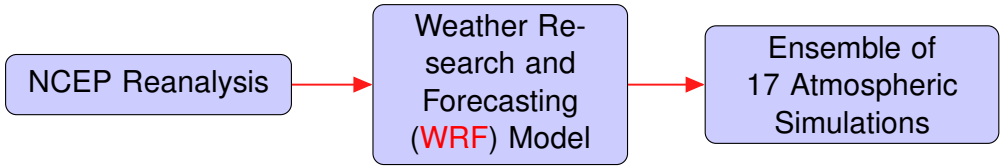
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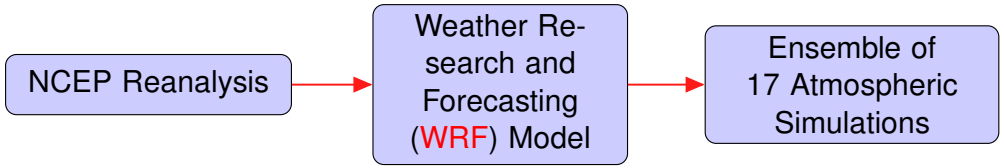
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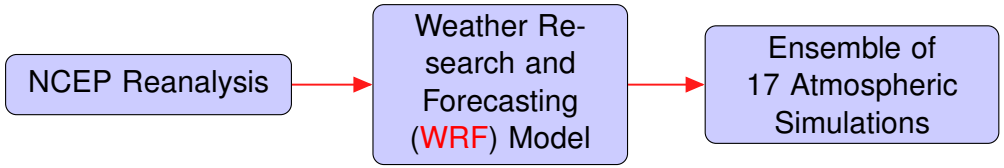


- Forward Modeling

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Numerical Experiement

- Atmospheric Simulation

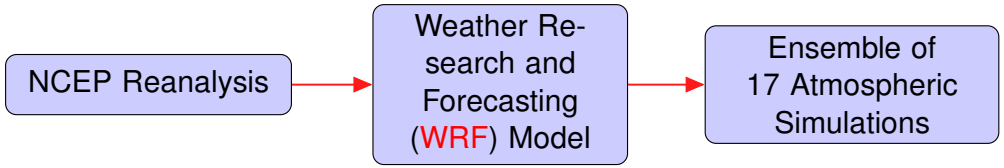


- Forward Modeling
  - Species: Xe-133.

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Numerical Experiement

- Atmospheric Simulation



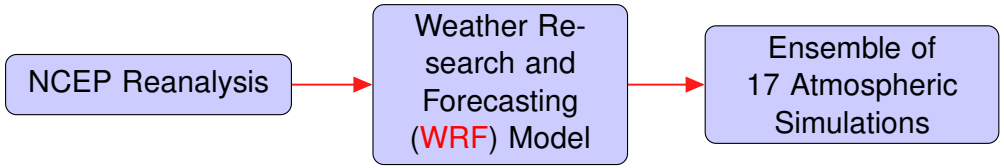
- Forward Modeling
  - Species: Xe-133.
  - Six sources are assumed.

Exp. ID	Location		Time of release
	Lat.	Lon.	
LOC1	46.47	-119.33	9 Oct. 6–12UTC
LOC2	37.12	-116.19	8 Oct. 6–12UTC
LOC3	34.62	-102.63	7 Oct. 6–12UTC
LOC4	34.70	-87.12	9 Oct. 6–12UTC
LOC5	39.62	-94.63	8 Oct. 6–12UTC
LOC6	39.62	-112.63	7 Oct. 6–12UTC

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Numerical Experiement

- Atmospheric Simulation

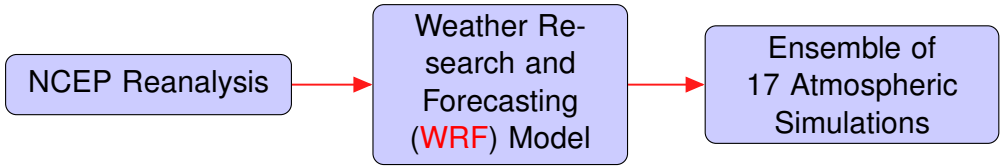


- Forward Modeling
  - Species: Xe-133.
  - Six sources are assumed.
  - three receptors(RN44, RN74, and RN75)

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Numerical Experiement

- Atmospheric Simulation



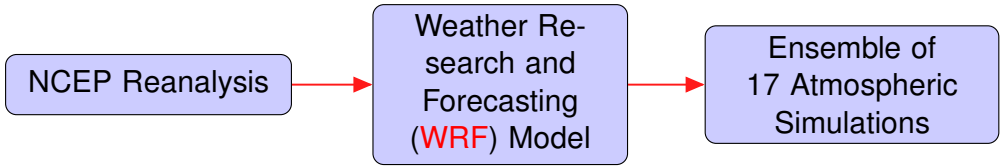
- Forward Modeling
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  - Six sources are assumed.
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Station ID	Lat.	Lon.
RN75	37.996	-78.399
RN74	37.167	-99.769
RN44	27.957	-114.063

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Numerical Experiement

- Atmospheric Simulation

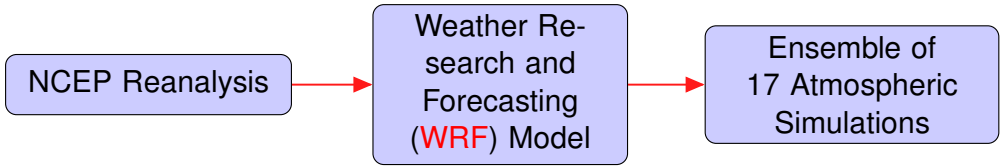


- Forward Modeling
  - Species: Xe-133.
  - Six sources are assumed.
  - three receptors(RN44, RN74, and RN75)
  - vertical Elevation: 0m and 100m above ground.

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Numerical Experiement

- Atmospheric Simulation

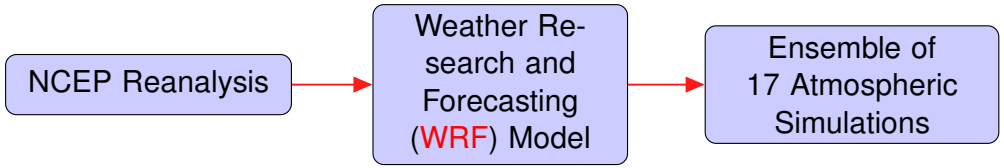


- Forward Modeling
  - Species: Xe-133.
  - Six sources are assumed.
  - three receptors(RN44, RN74, and RN75)
  - vertical Elevation: 0m and 100m above ground.
  - Released Particles: 10000 particles with total mass of 1kg.

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Numerical Experiement

- Atmospheric Simulation



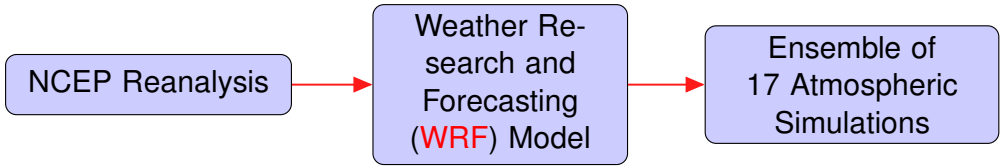
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  - vertical Elevation: 0m and 100m above ground.
  - Released Particles: 10000 particles with total mass of $1kg$.
  - total number of forward simulations

$$6 \quad \text{Sources} \times 17 \quad \text{ensemble members} = 102 \quad \text{Simulations}$$

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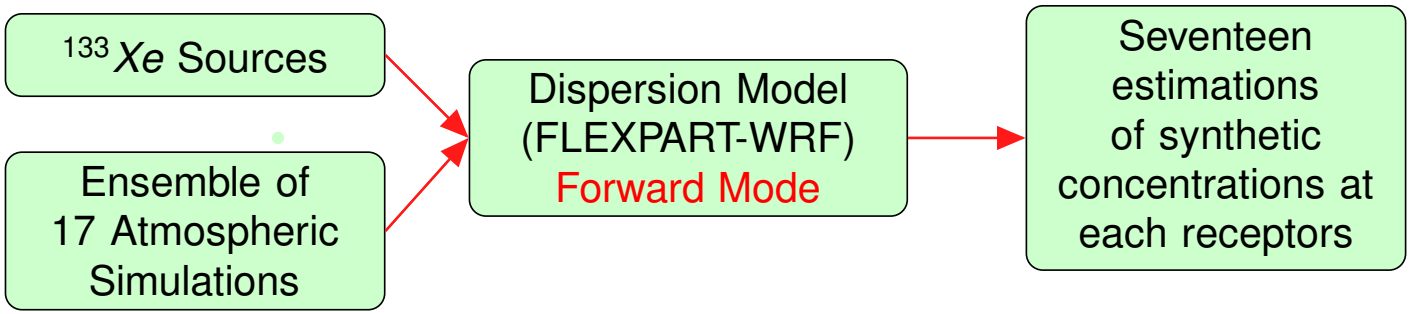
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- Atmospheric Simulation



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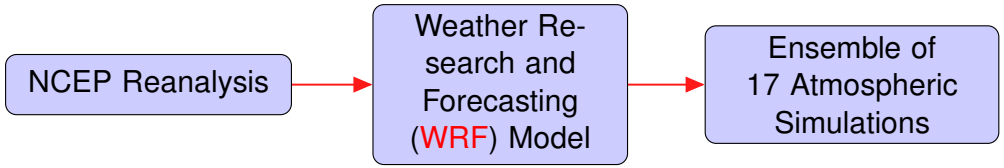
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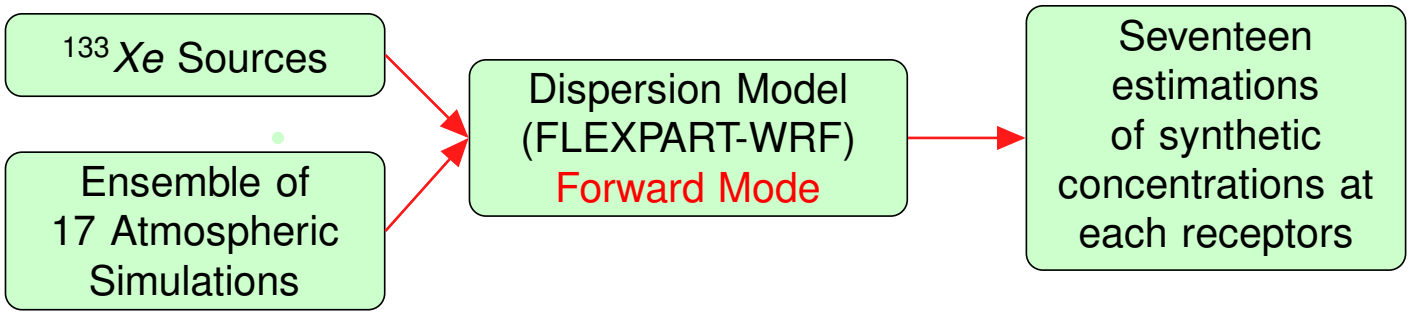
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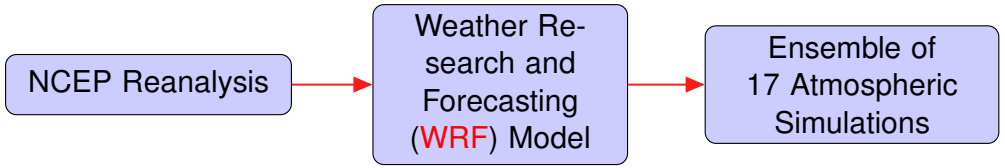
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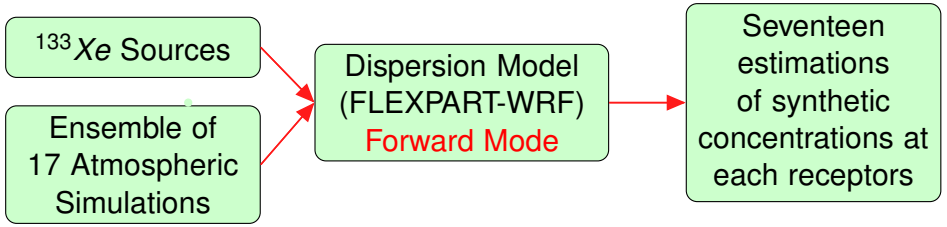
  - Synthetic Samples Collection Time: 24 hours.

Numerical Experiement

- Atmospheric Simulation



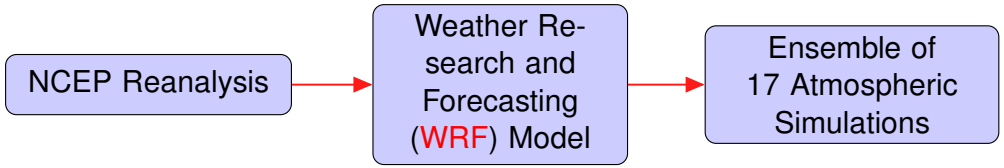
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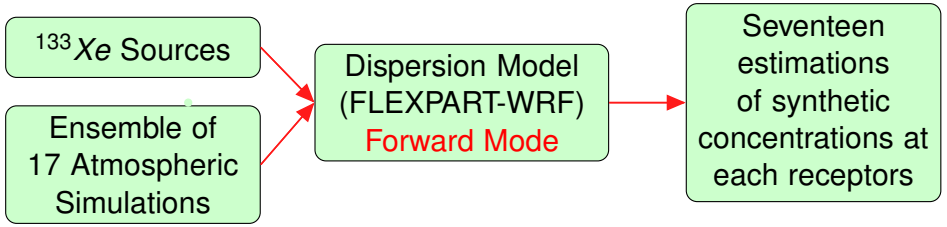
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Numerical Experiement

- Atmospheric Simulation



- Forward Modeling

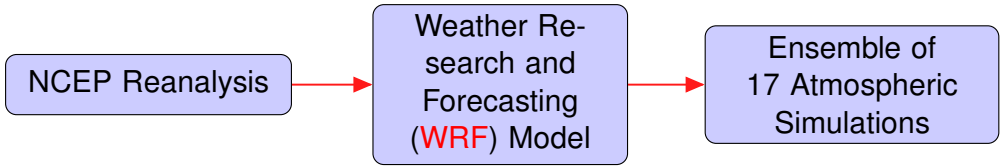


- Adjoint Modeling

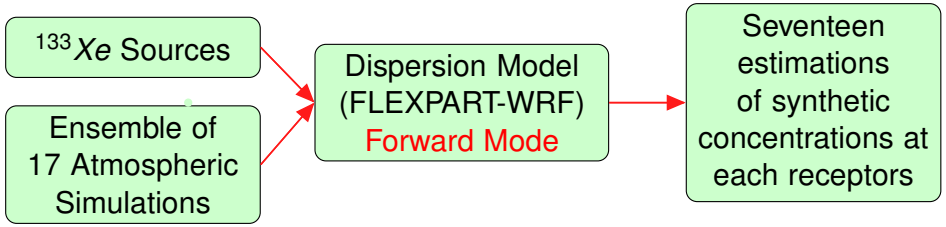
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Numerical Experiement

- Atmospheric Simulation



- Forward Modeling

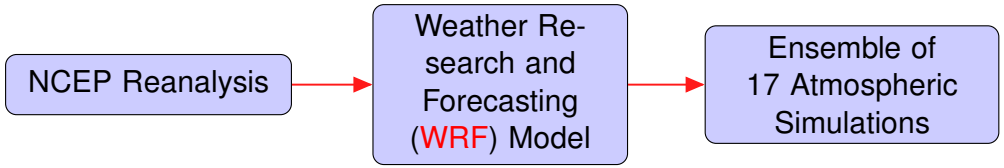


- Adjoint Modeling
  - Retroplumes begin from IMS stations (RN44,RN74,RN75)

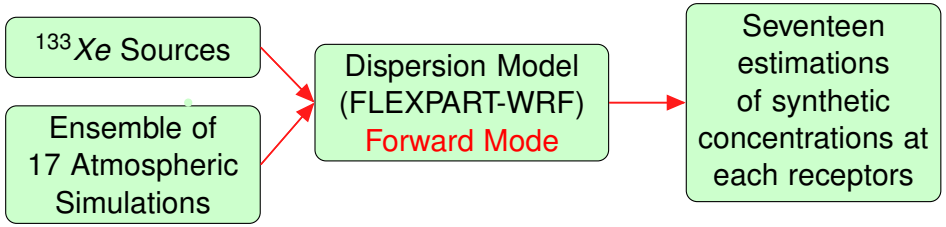
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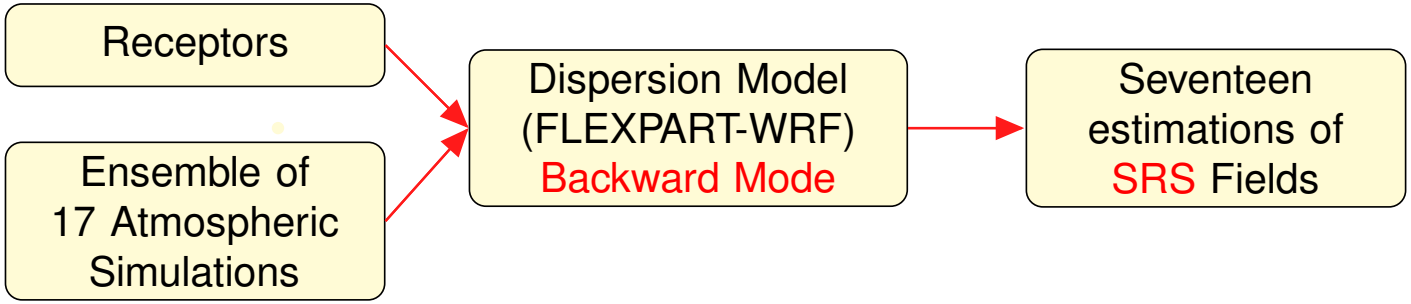
- Atmospheric Simulation



- Forward Modeling



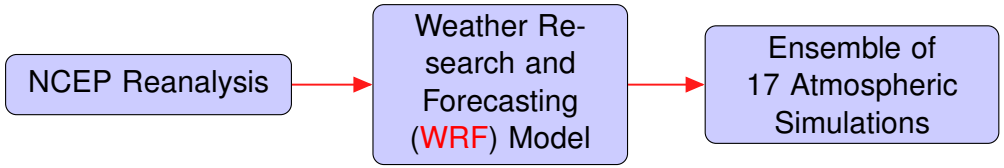
- Adjoint Modeling
  - Retroplumes begin from IMS stations (RN44,RN74,RN75)



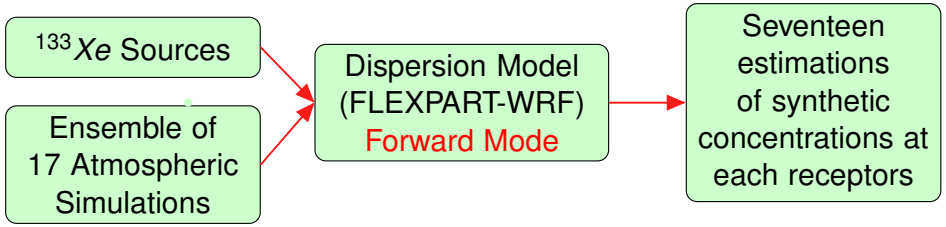
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Numerical Experiement

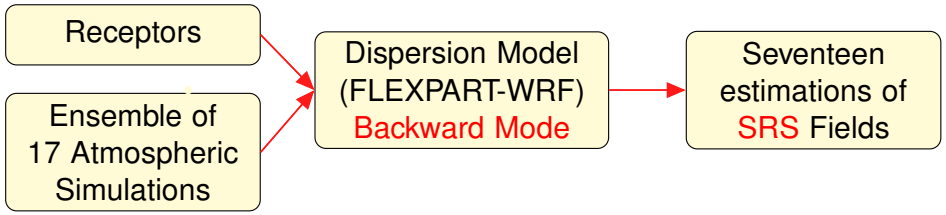
- Atmospheric Simulation



- Forward Modeling



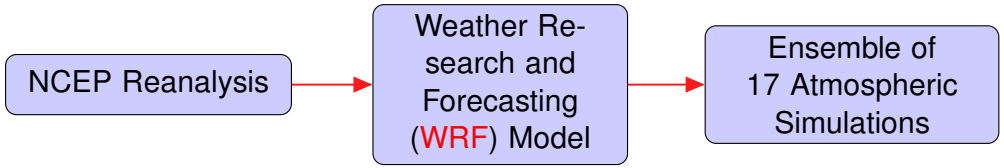
- Adjoint Modeling



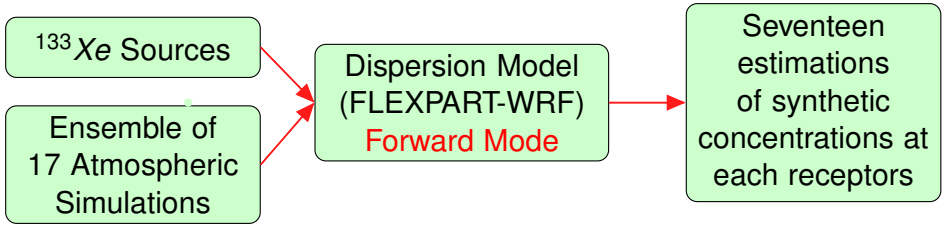
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Numerical Experiement

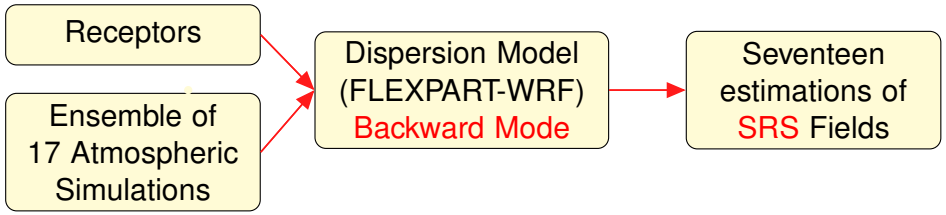
- Atmospheric Simulation



- Forward Modeling



- Adjoint Modeling

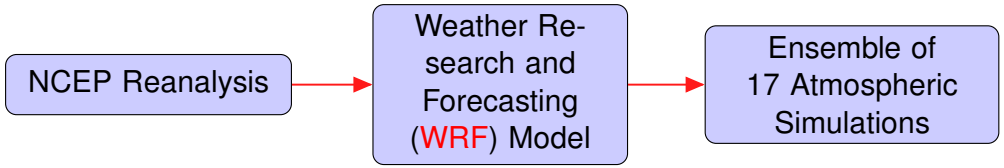


- Inverse Modeling

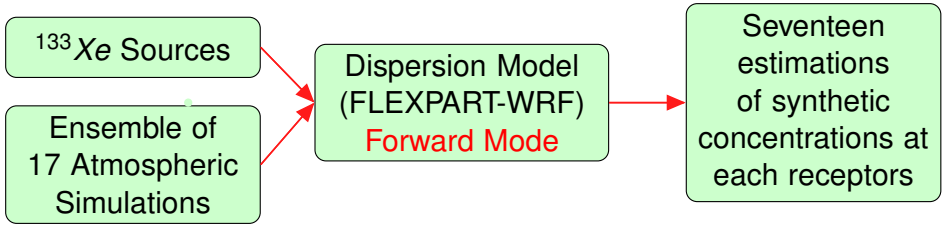
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Numerical Experiement

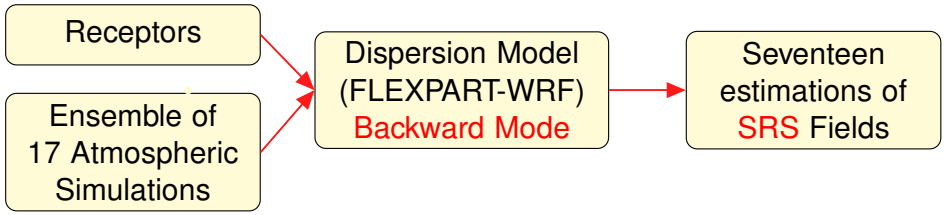
- Atmospheric Simulation



- Forward Modeling



- Adjoint Modeling

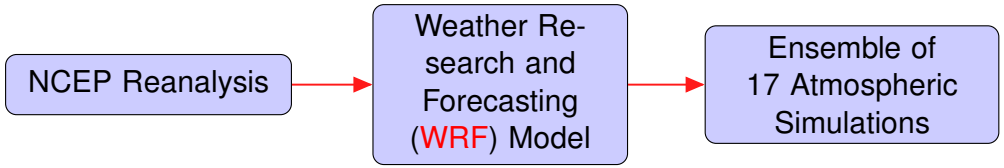


- Inverse Modeling
  - Source's Prior Assumptions:

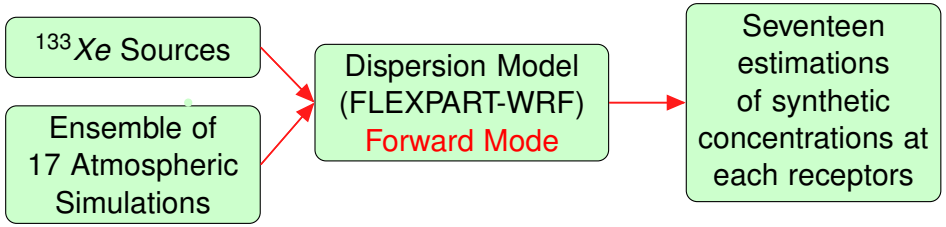
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Numerical Experiement

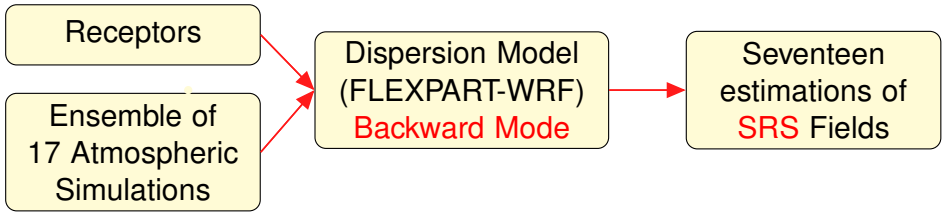
- Atmospheric Simulation



- Forward Modeling



- Adjoint Modeling

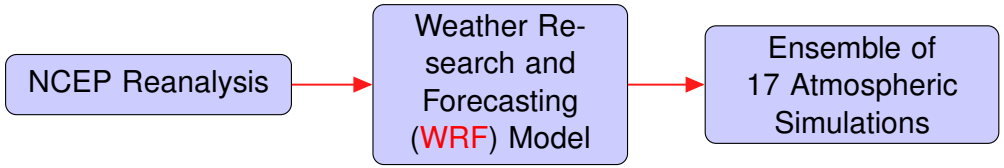


- Inverse Modeling
  - Source's Prior Assumptions:
    - the source is assumed to be located only at one grid cell.
    - the release occurs with constant rate during 24 hours.

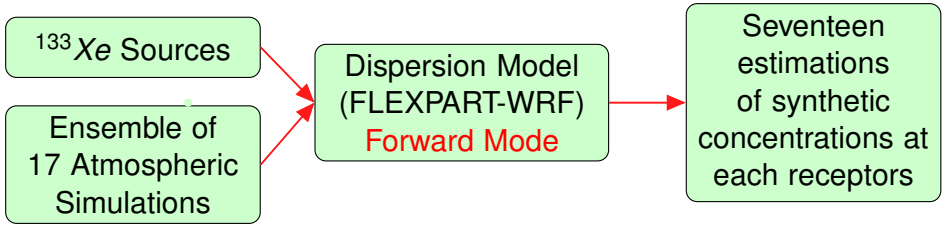
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Numerical Experiement

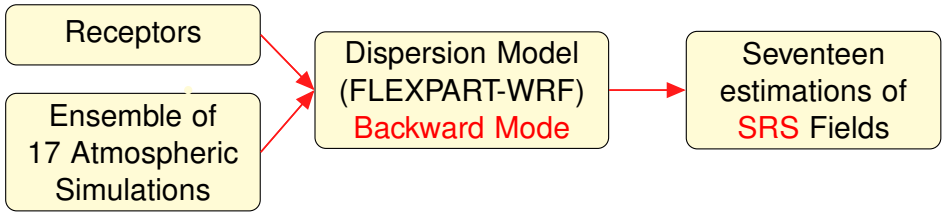
- Atmospheric Simulation



- Forward Modeling



- Adjoint Modeling



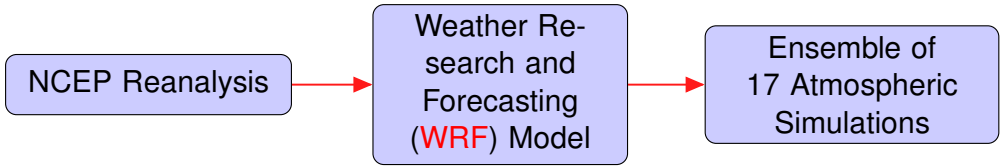
- Inverse Modeling
  - Source's Prior Assumptions:
  - Modeled Concentrations:

$$c_k = \sum M_{ijnk} S_{ijn}$$

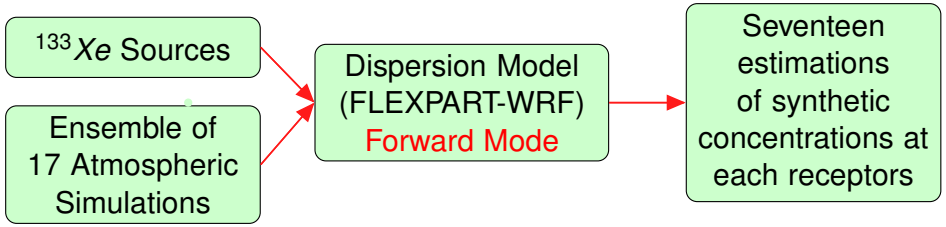
$$c_k^{obs} = AsM_{ijnk} + B$$

Numerical Experiement

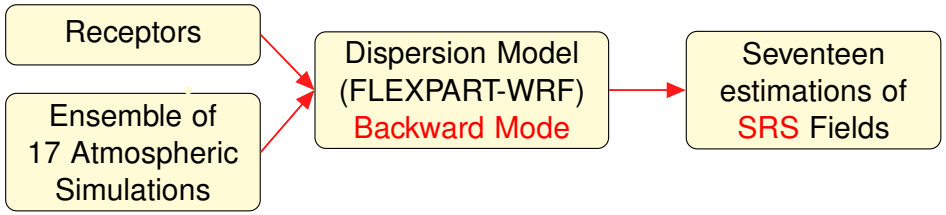
- Atmospheric Simulation



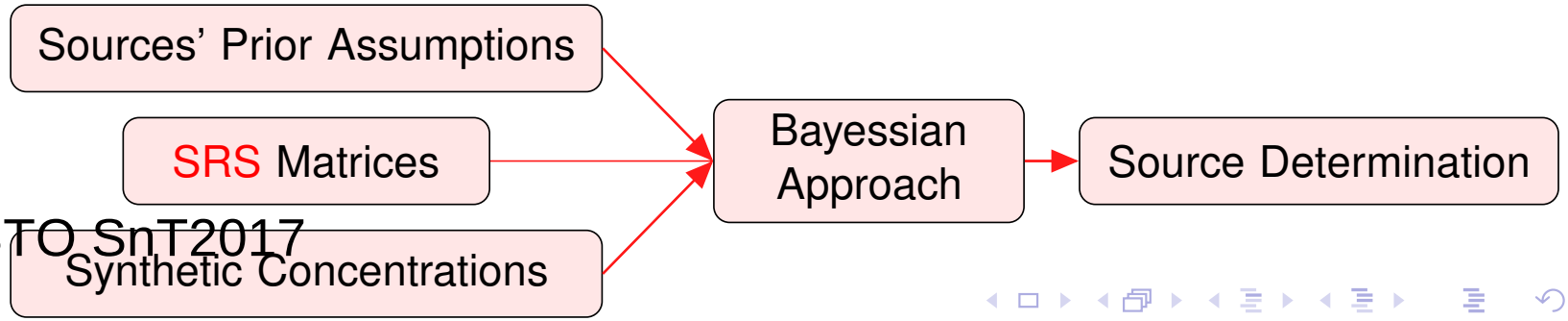
- Forward Modeling



- Adjoint Modeling

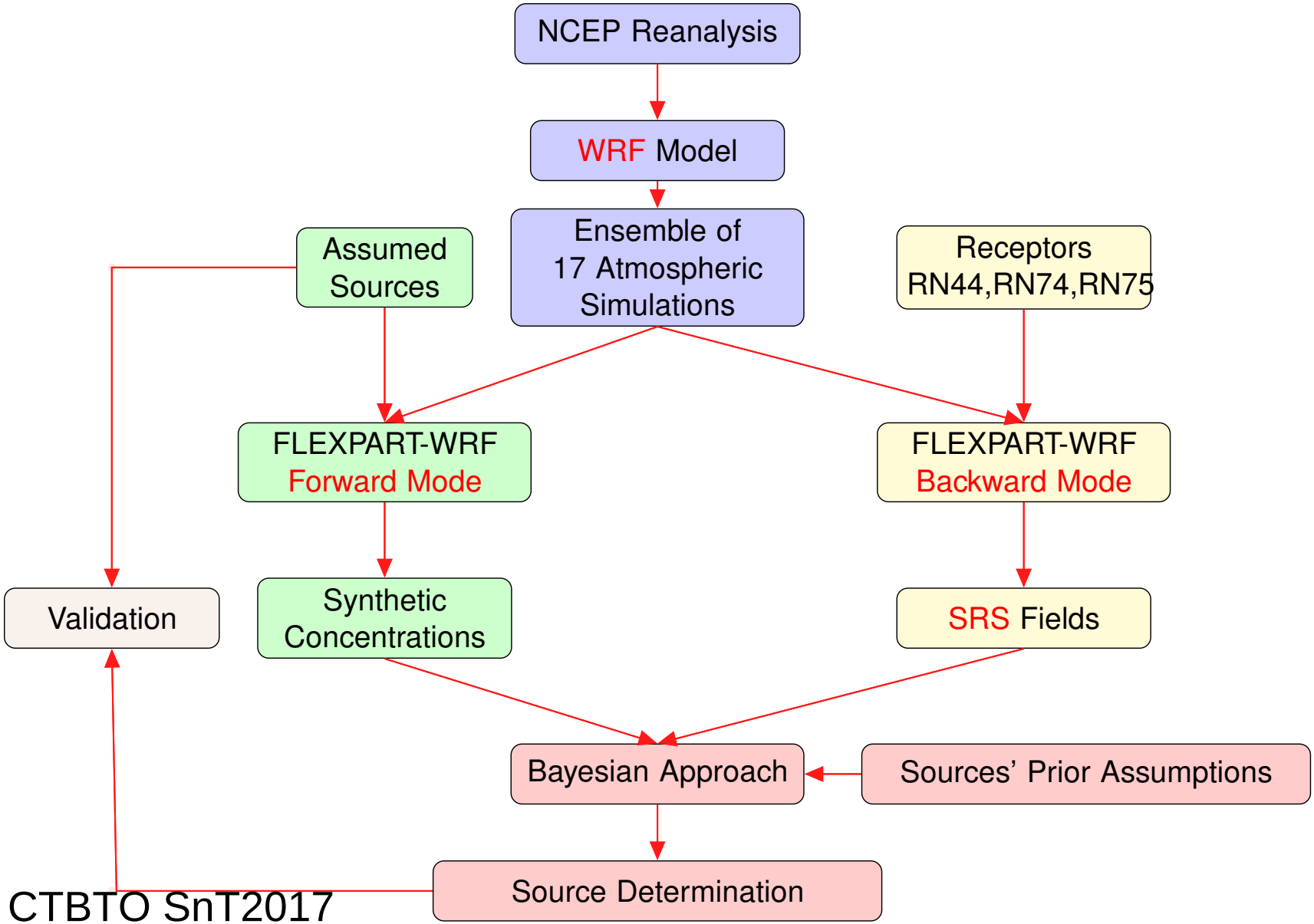


- Inverse Modeling



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Numerical Experiment



Results

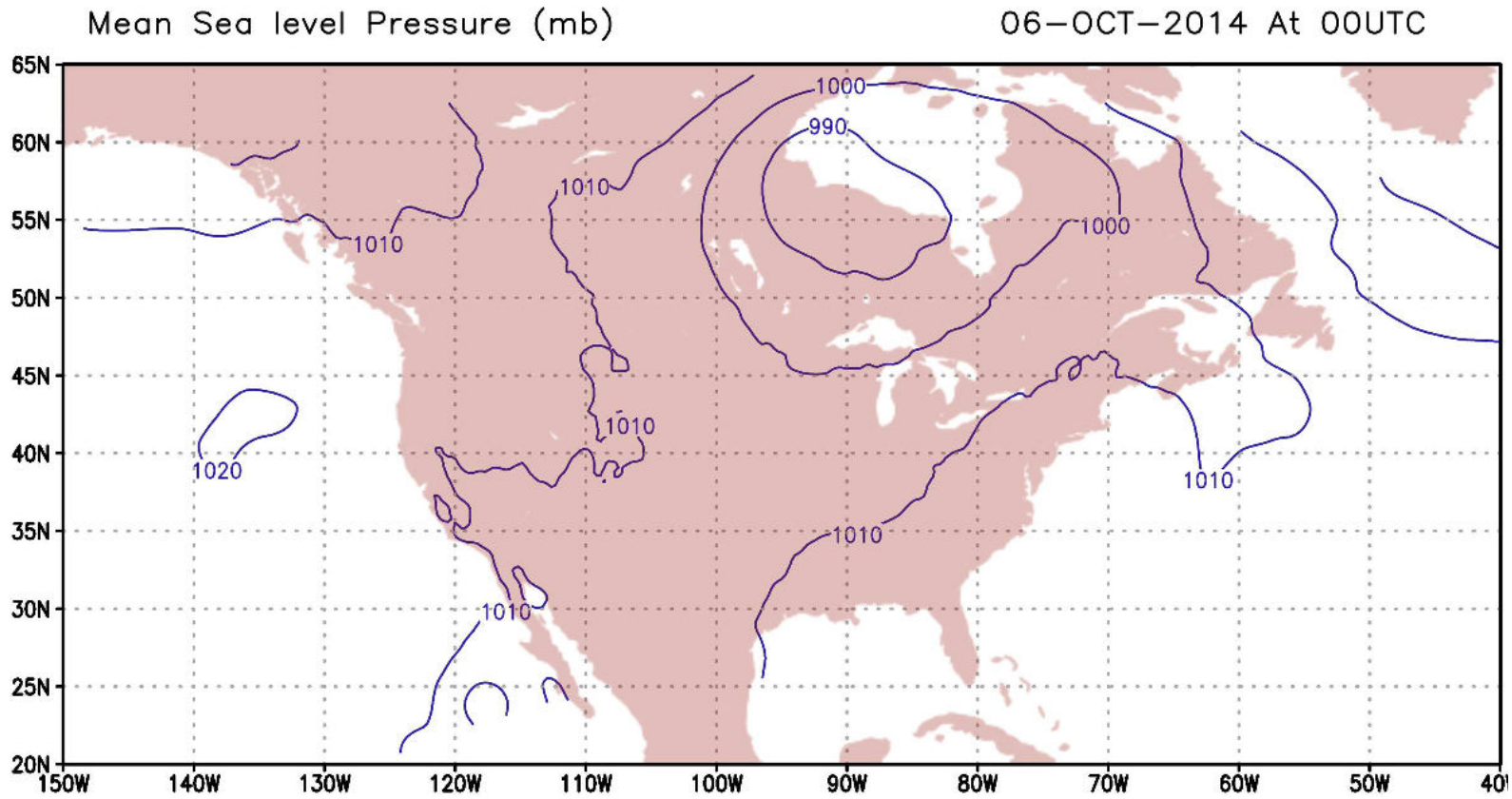
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Outline

1. Uncertainties in ATM modeling (An overview)
2. Configuration of a Numerical Experiment
3. Results
   - Uncertainties in Atmospheric Simulations
   - Uncertainties in Forward ATM
   - Sources Uncertainties Quantification
4. Conclusions

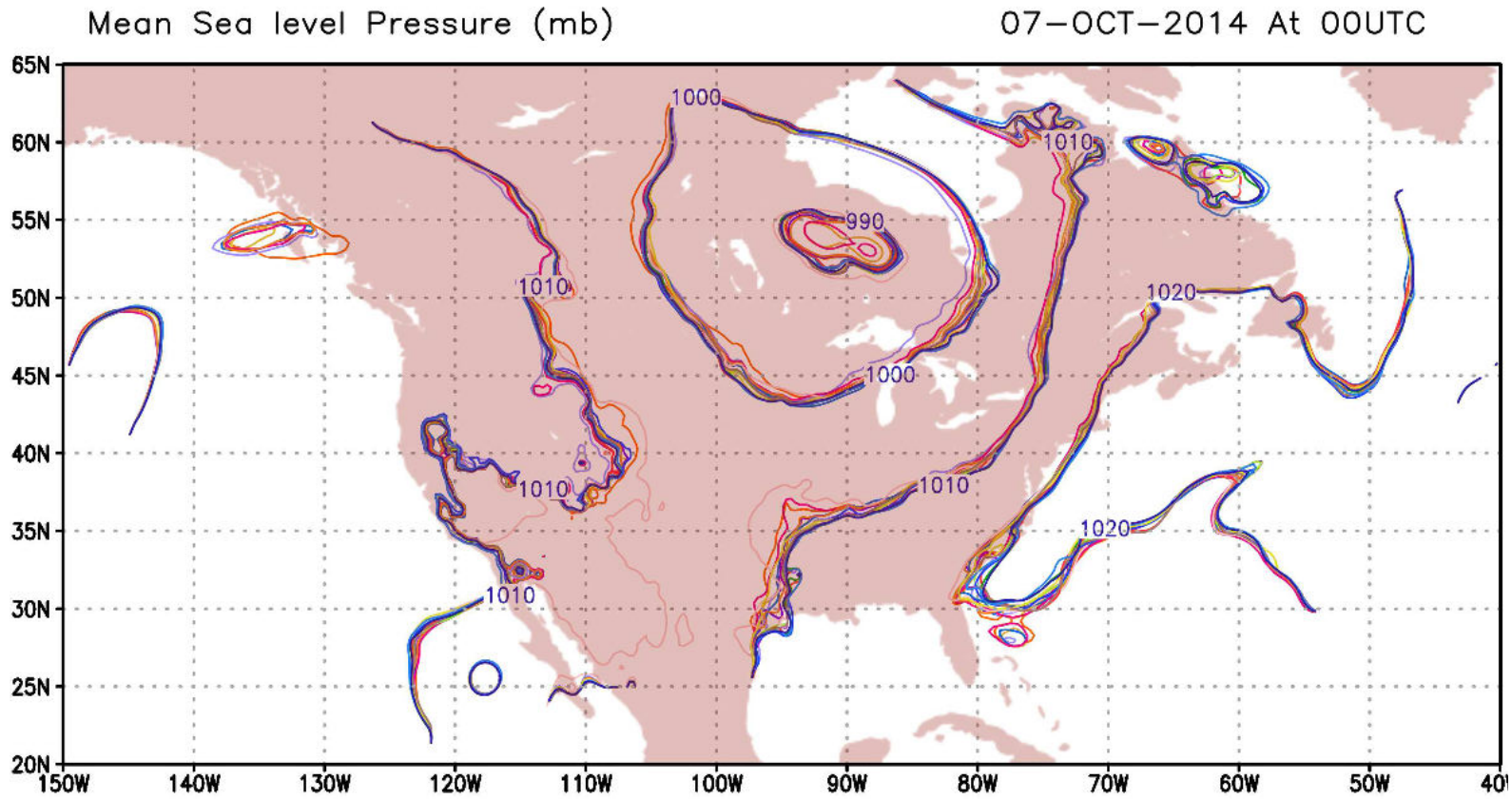
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Spagetti Charts (MSLP)



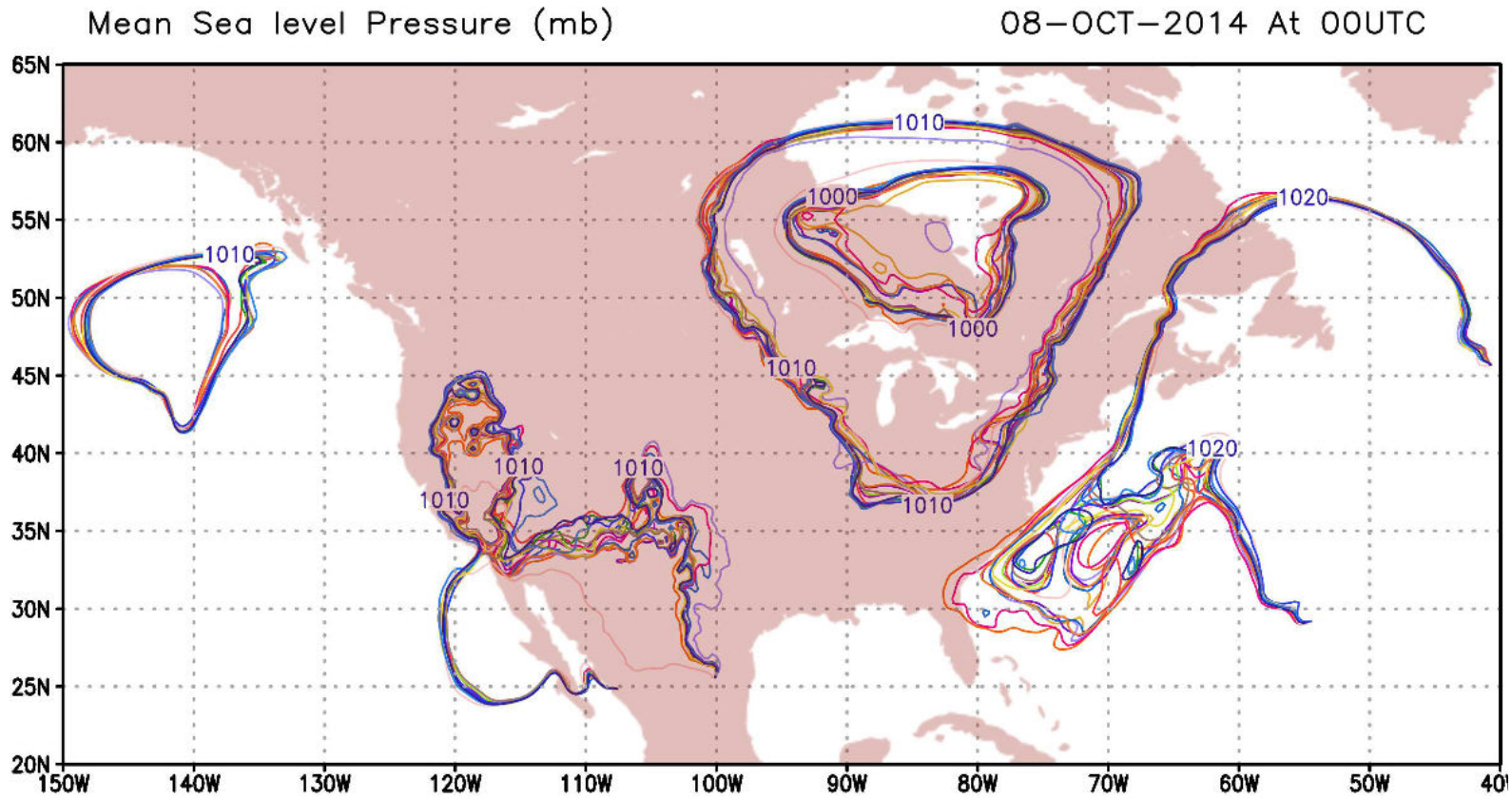
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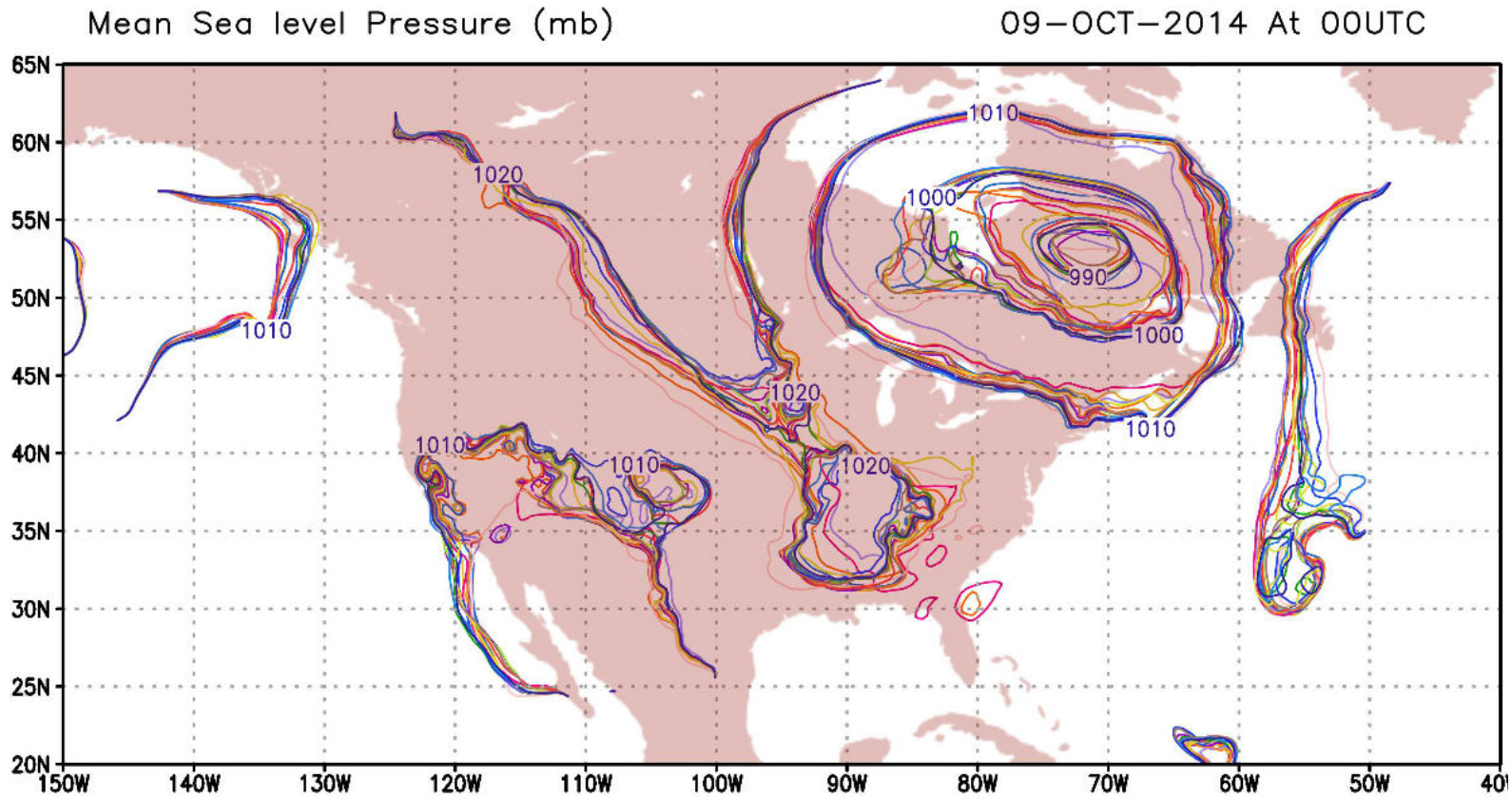
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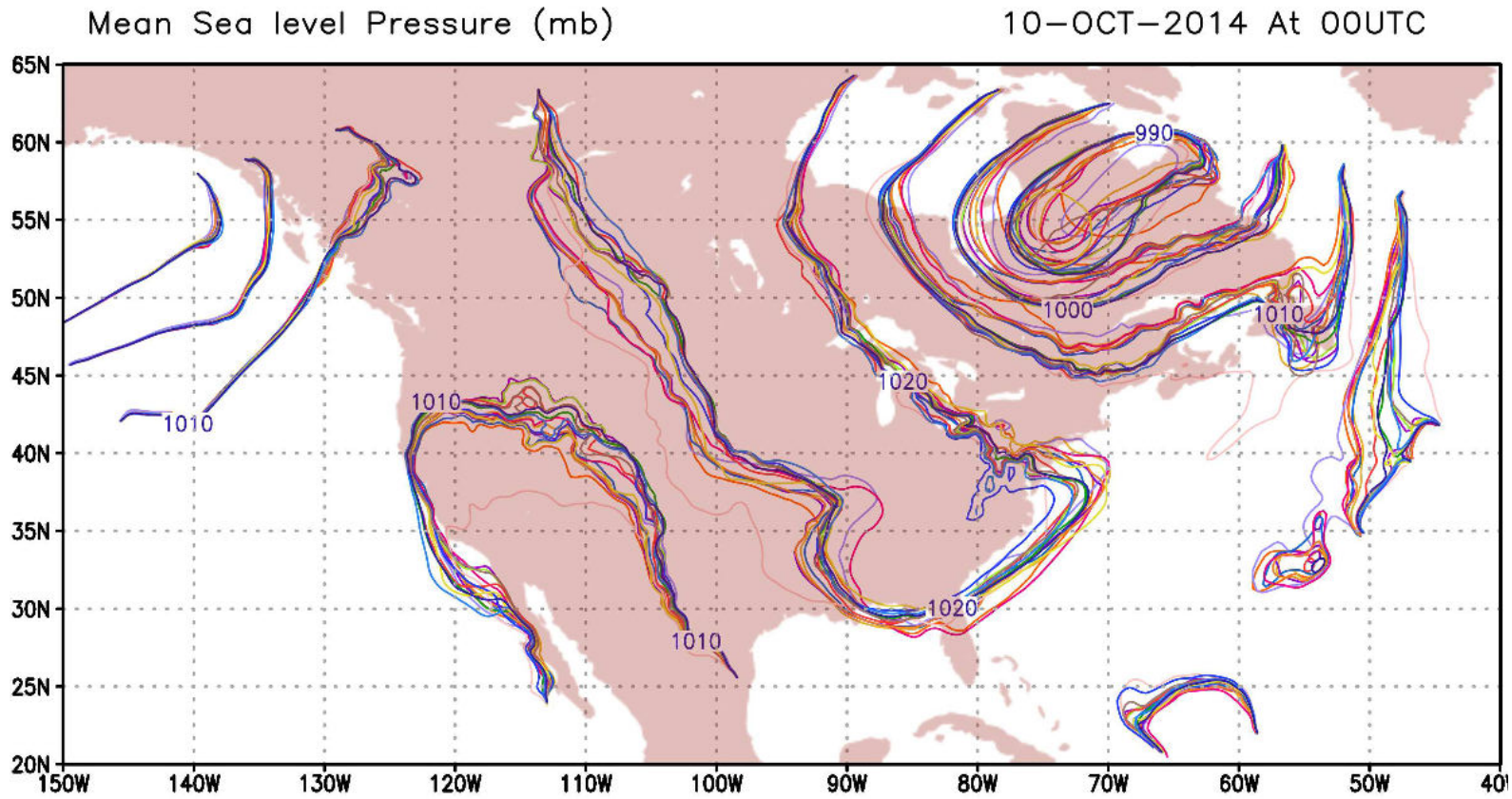
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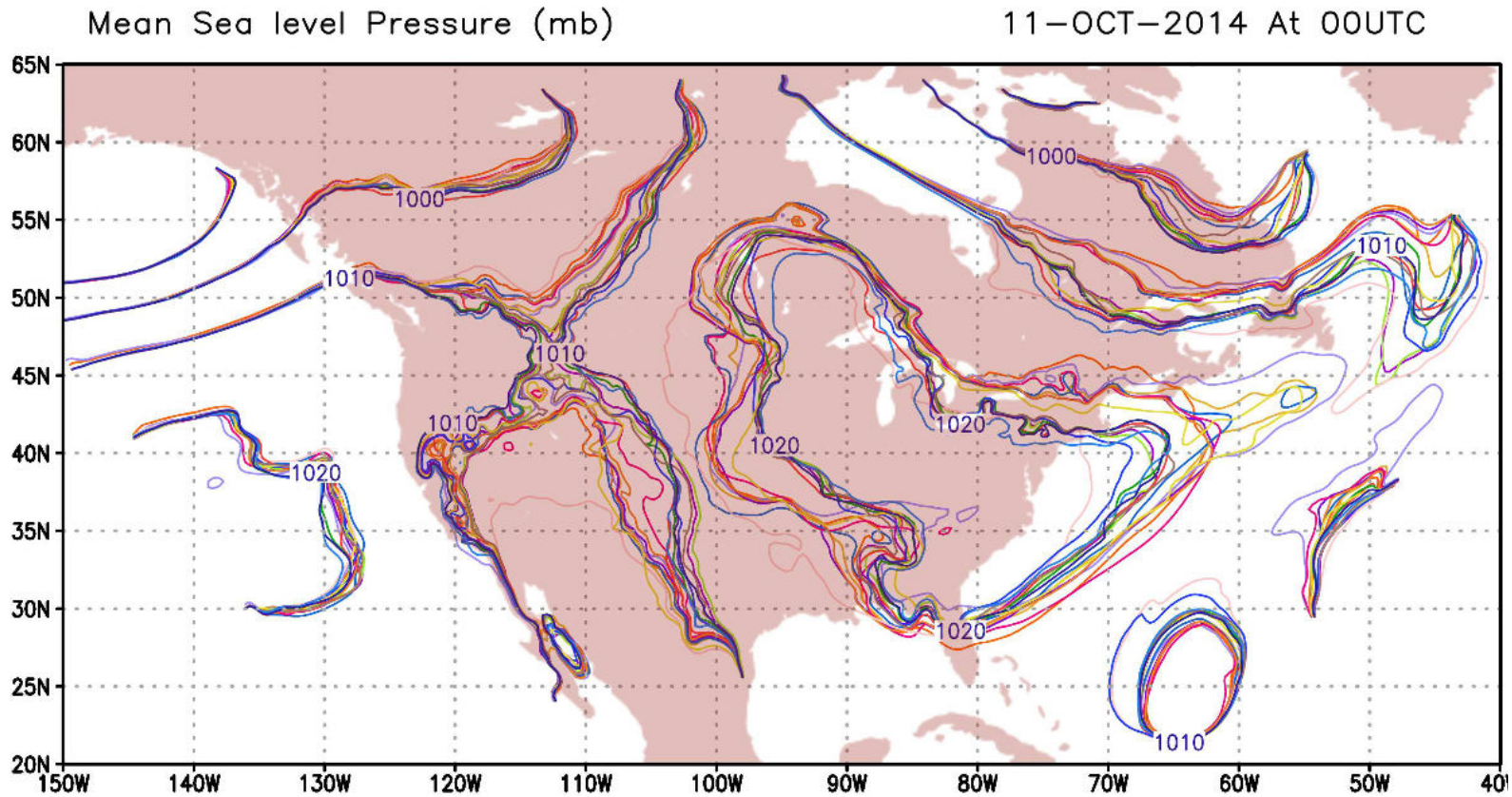
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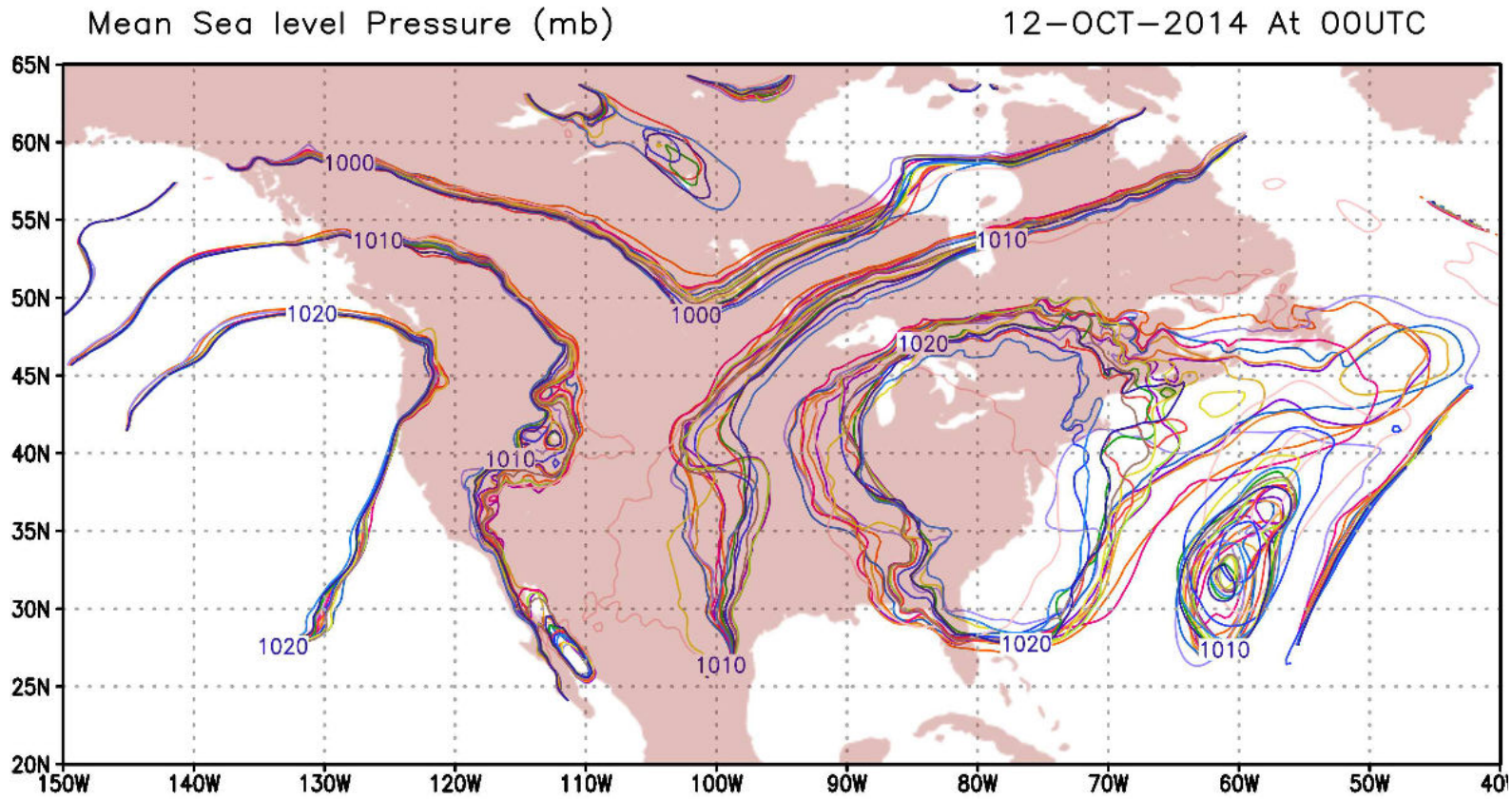
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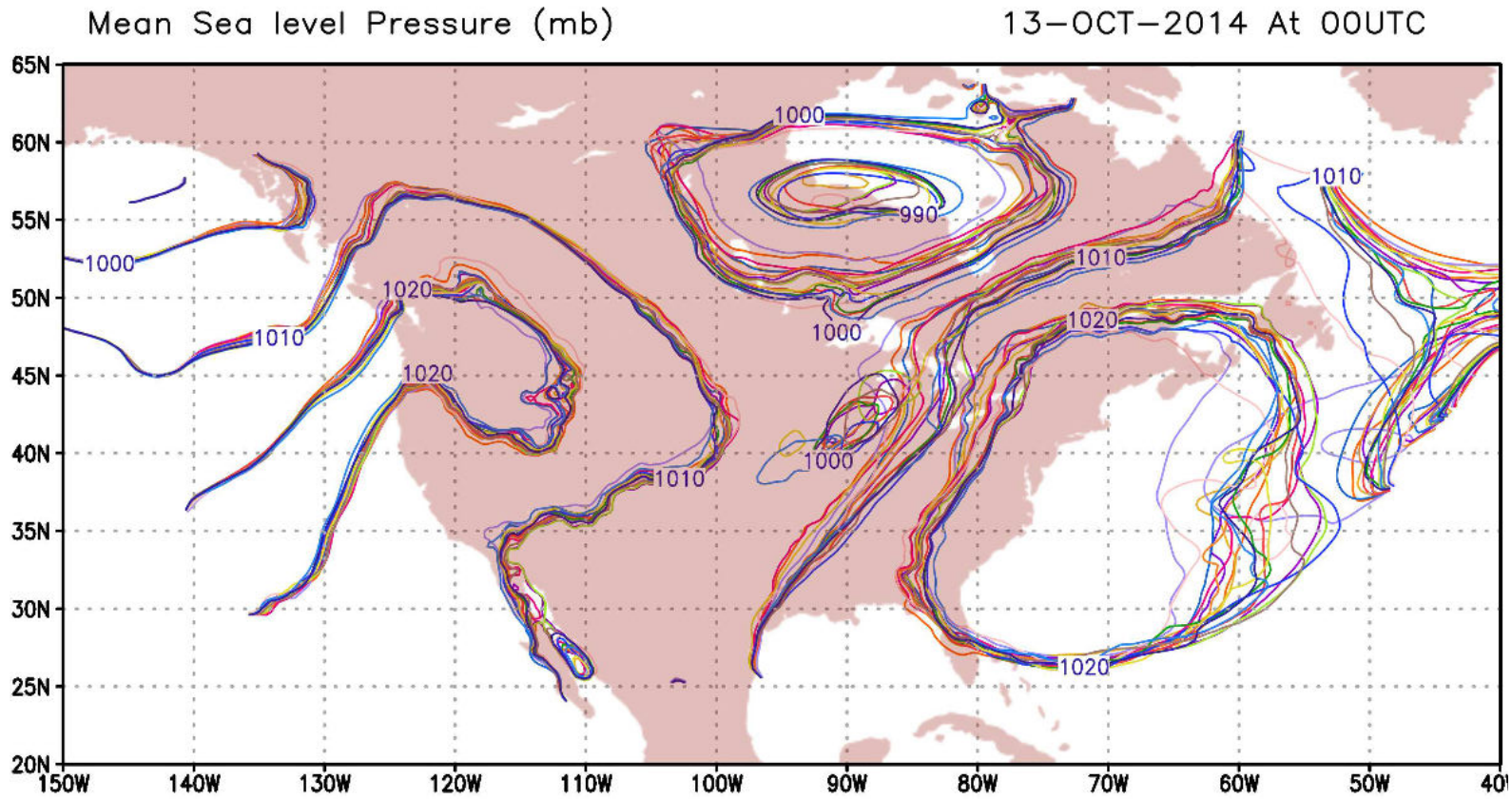
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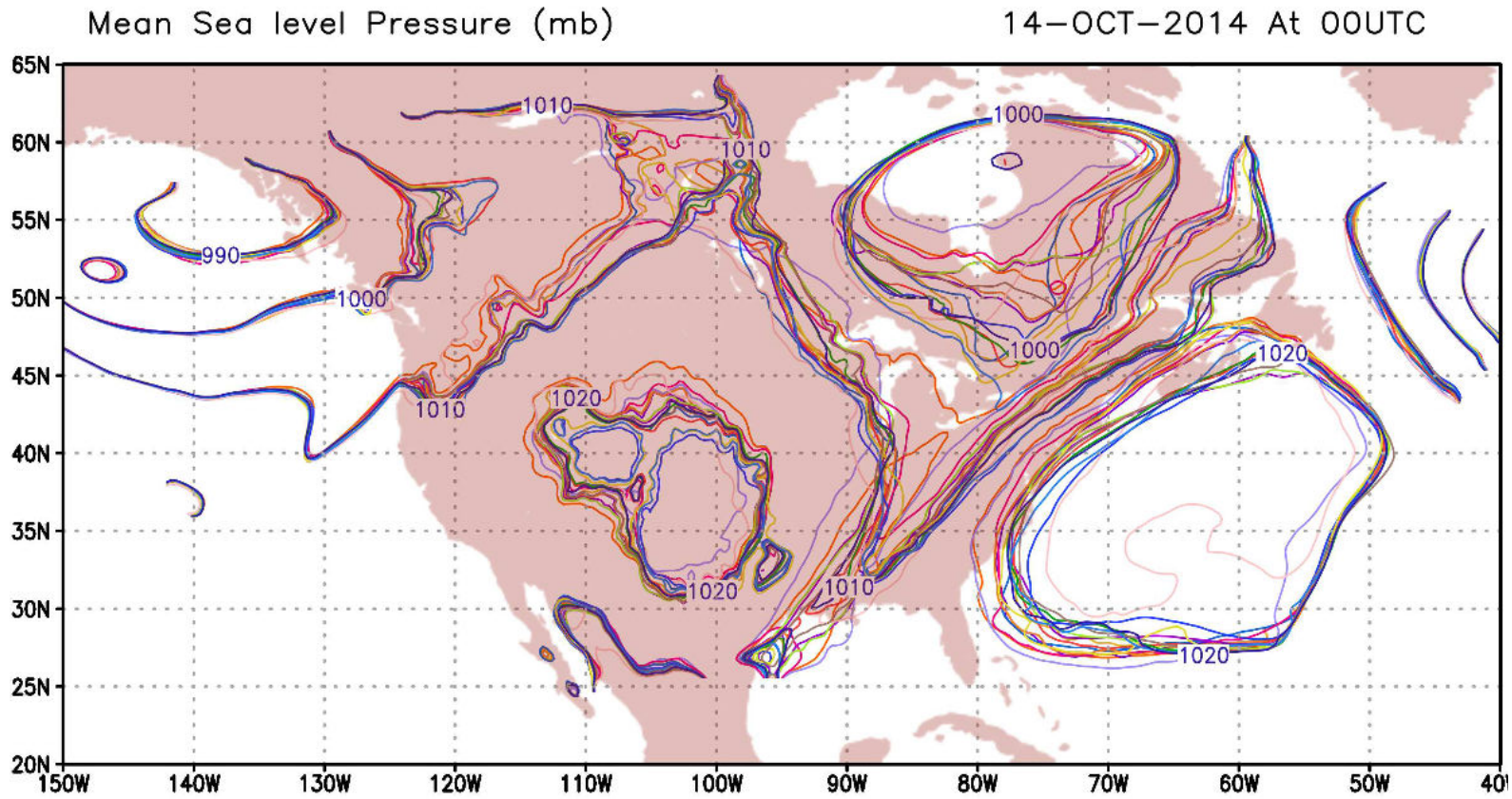
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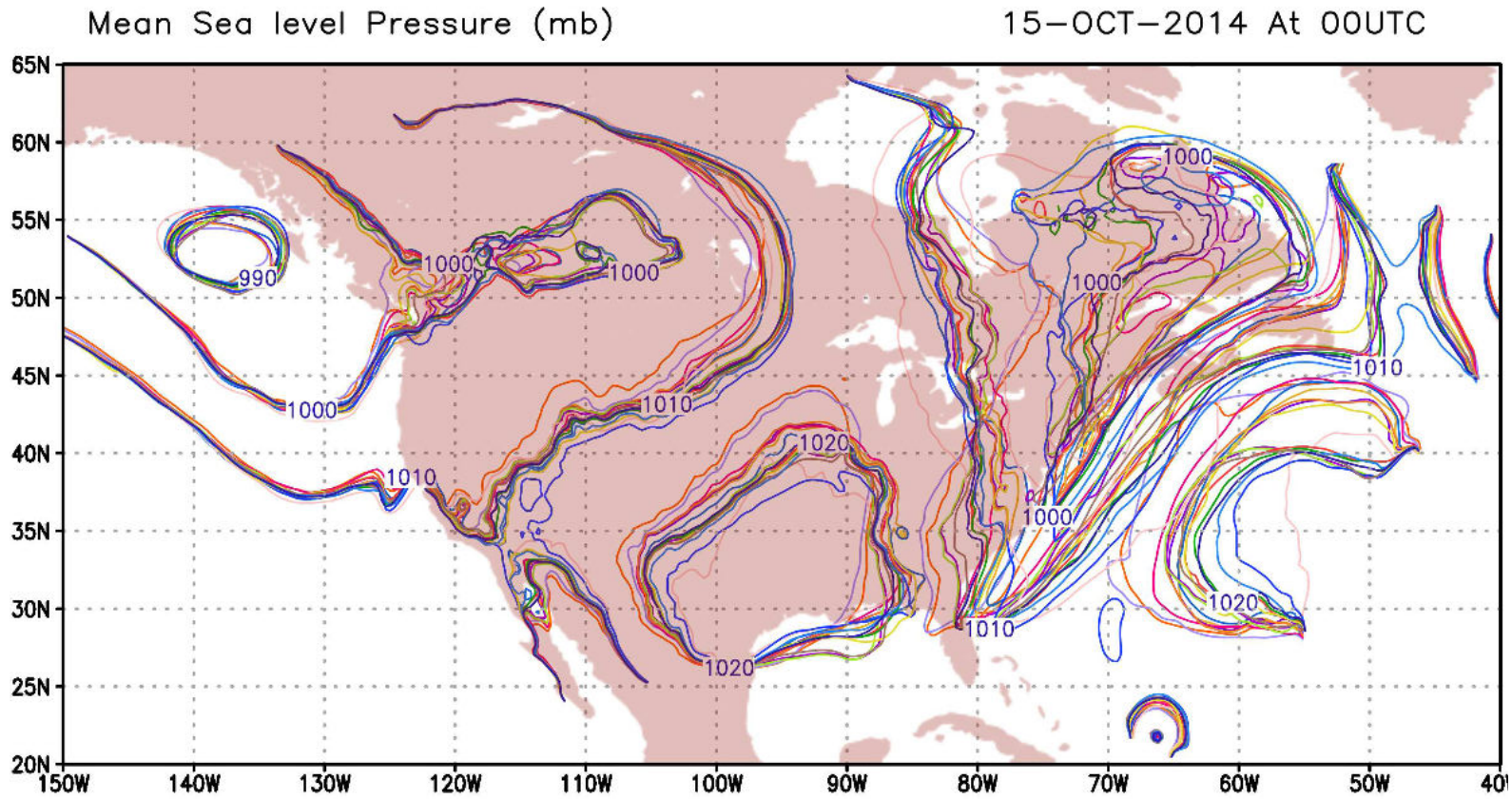
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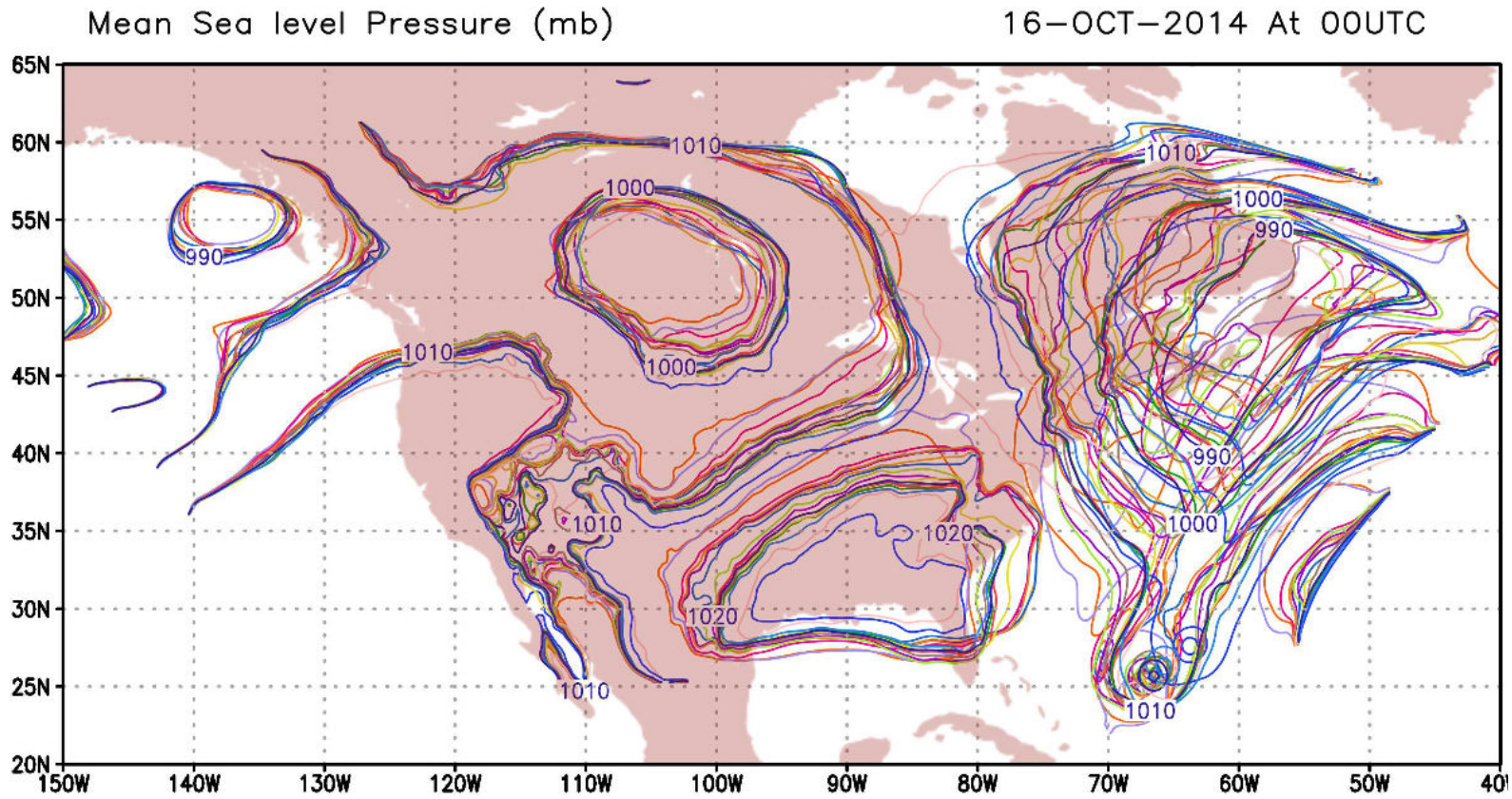
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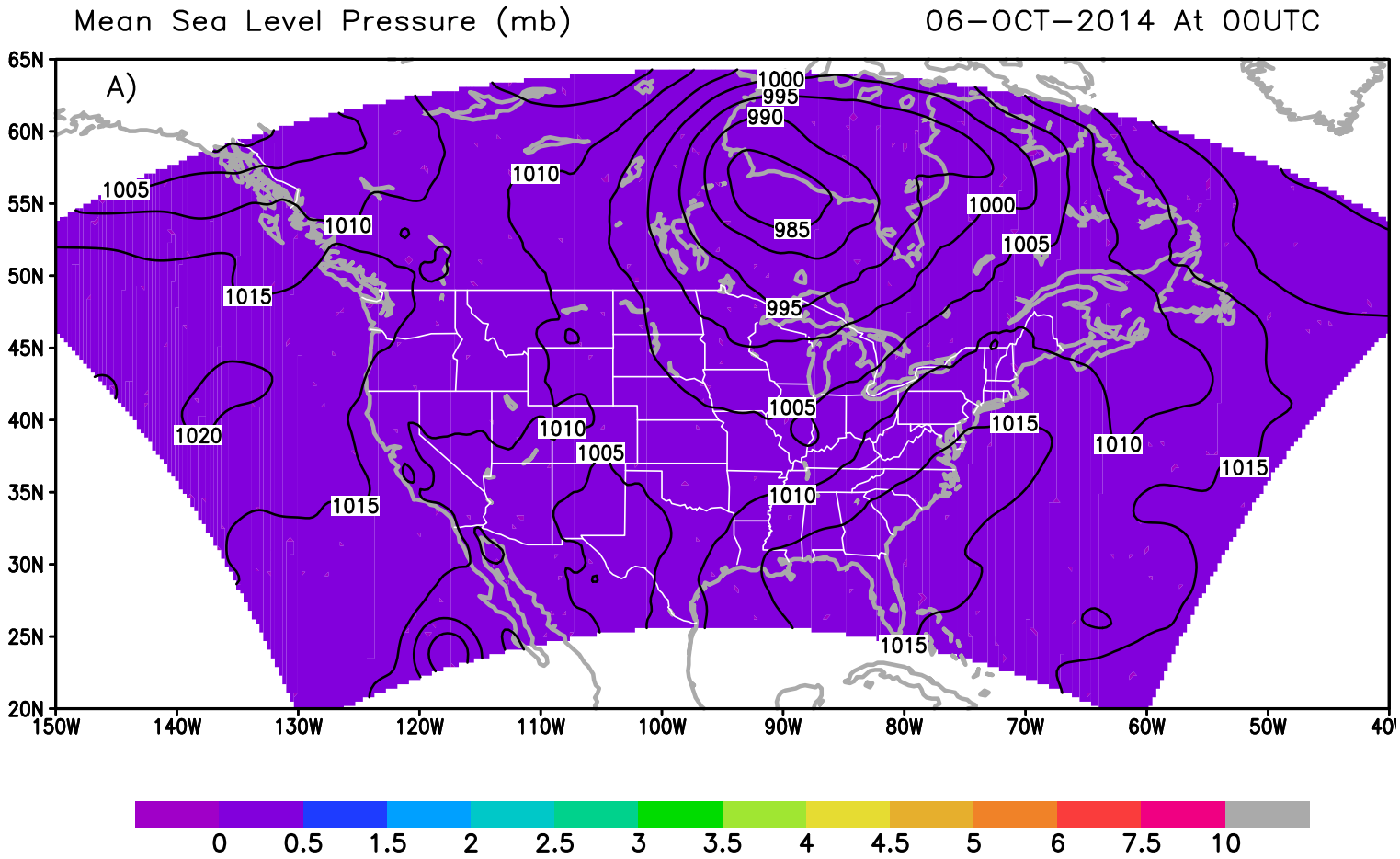
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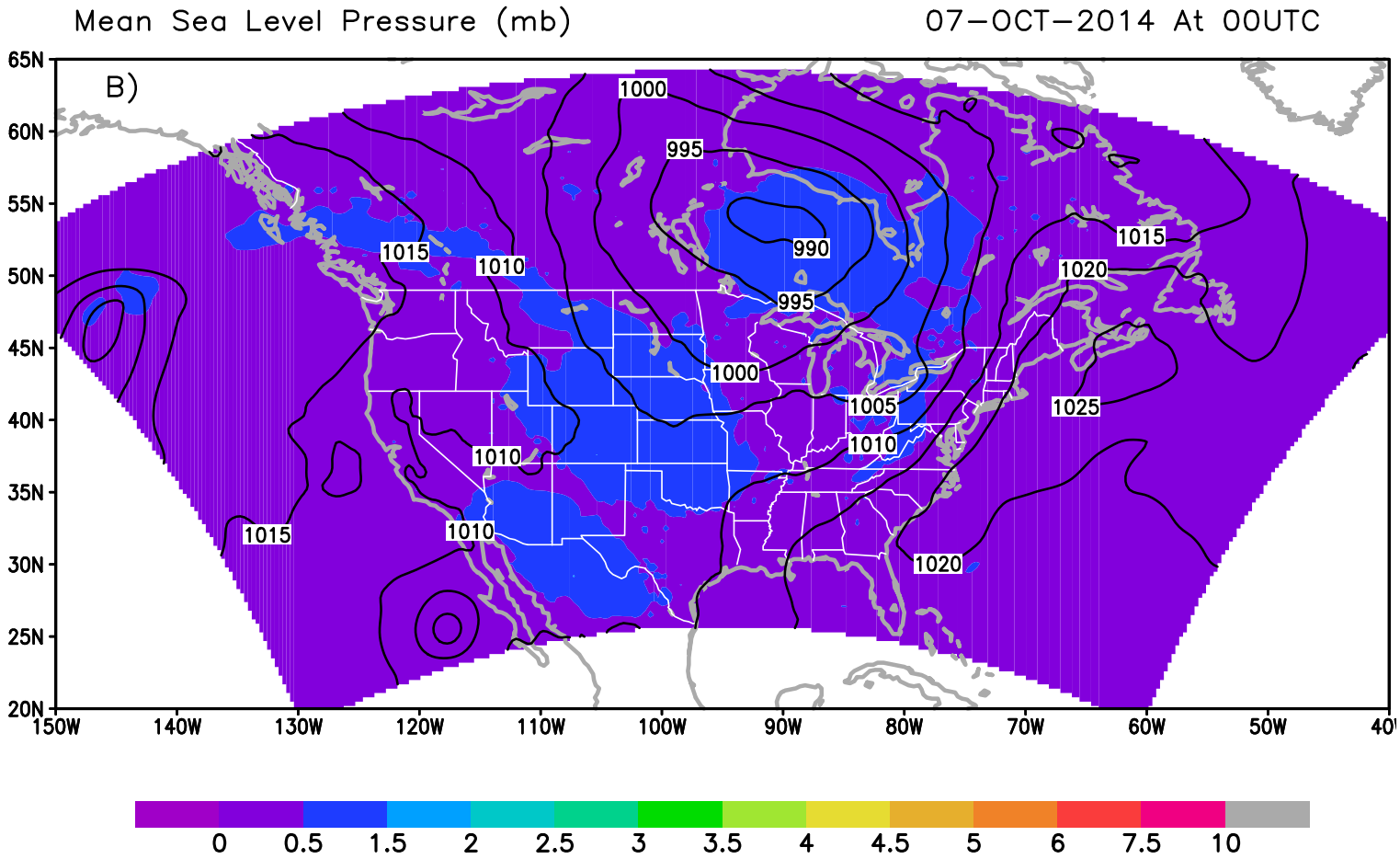
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Mean–Variance Charts (MSLP)



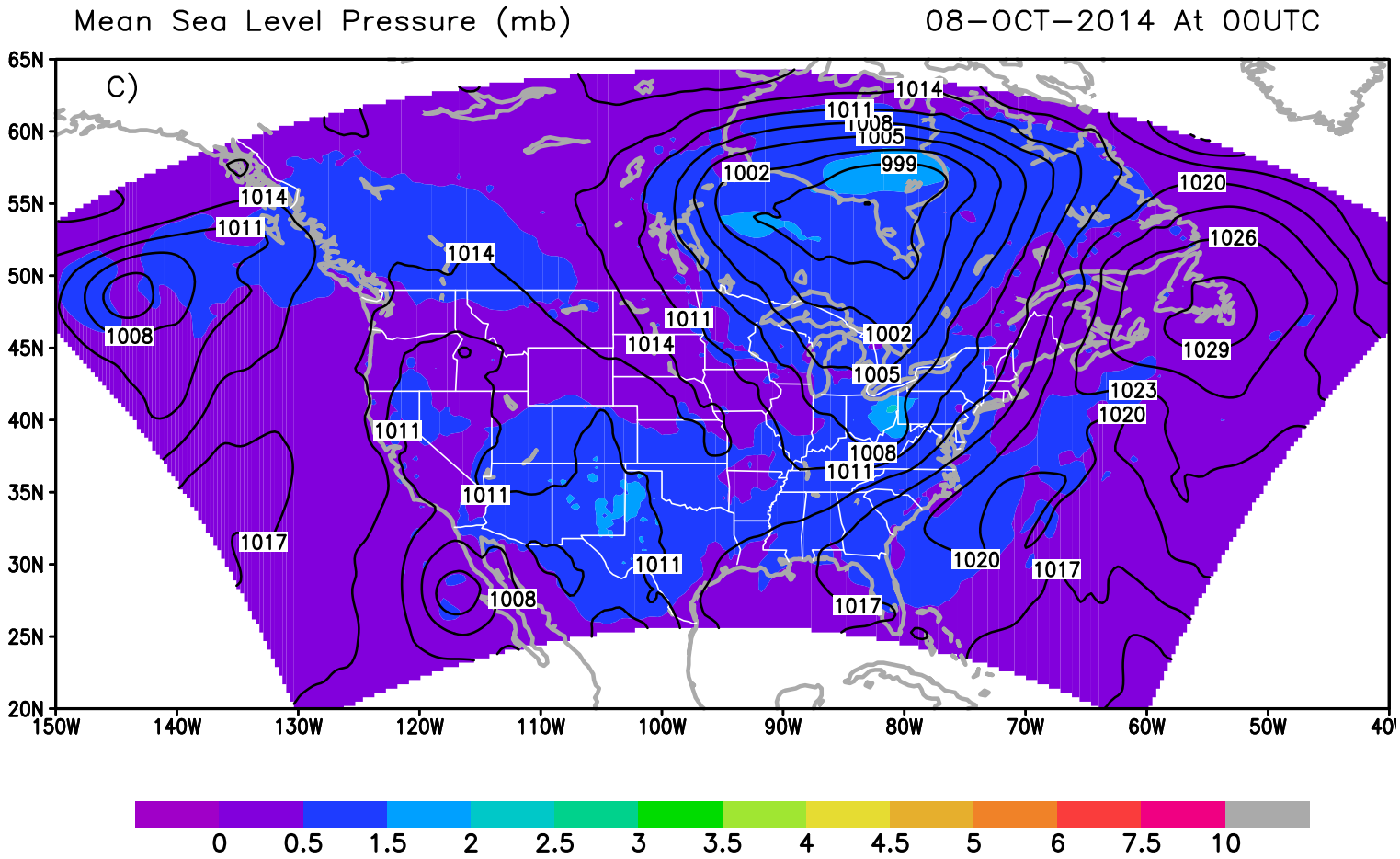
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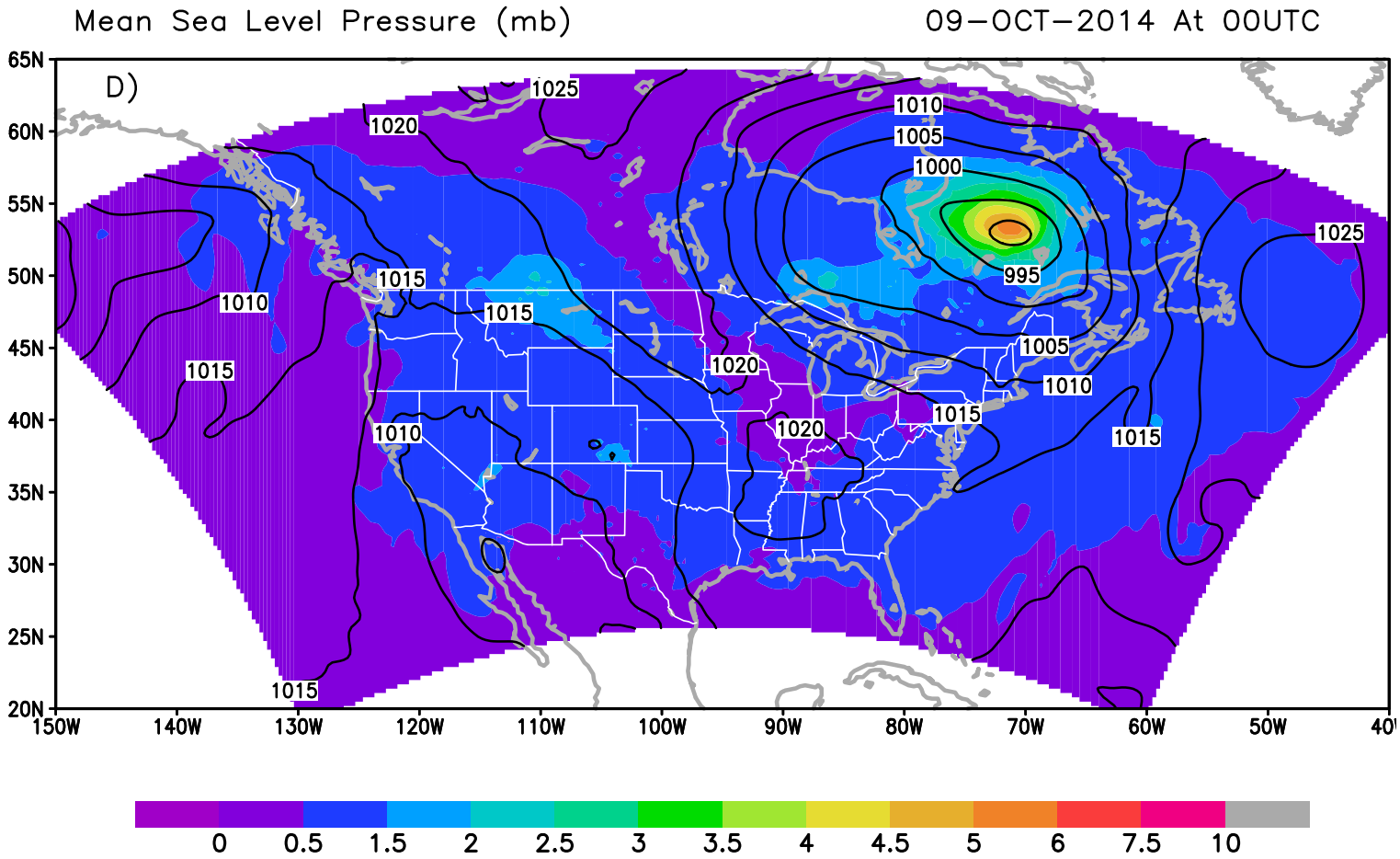
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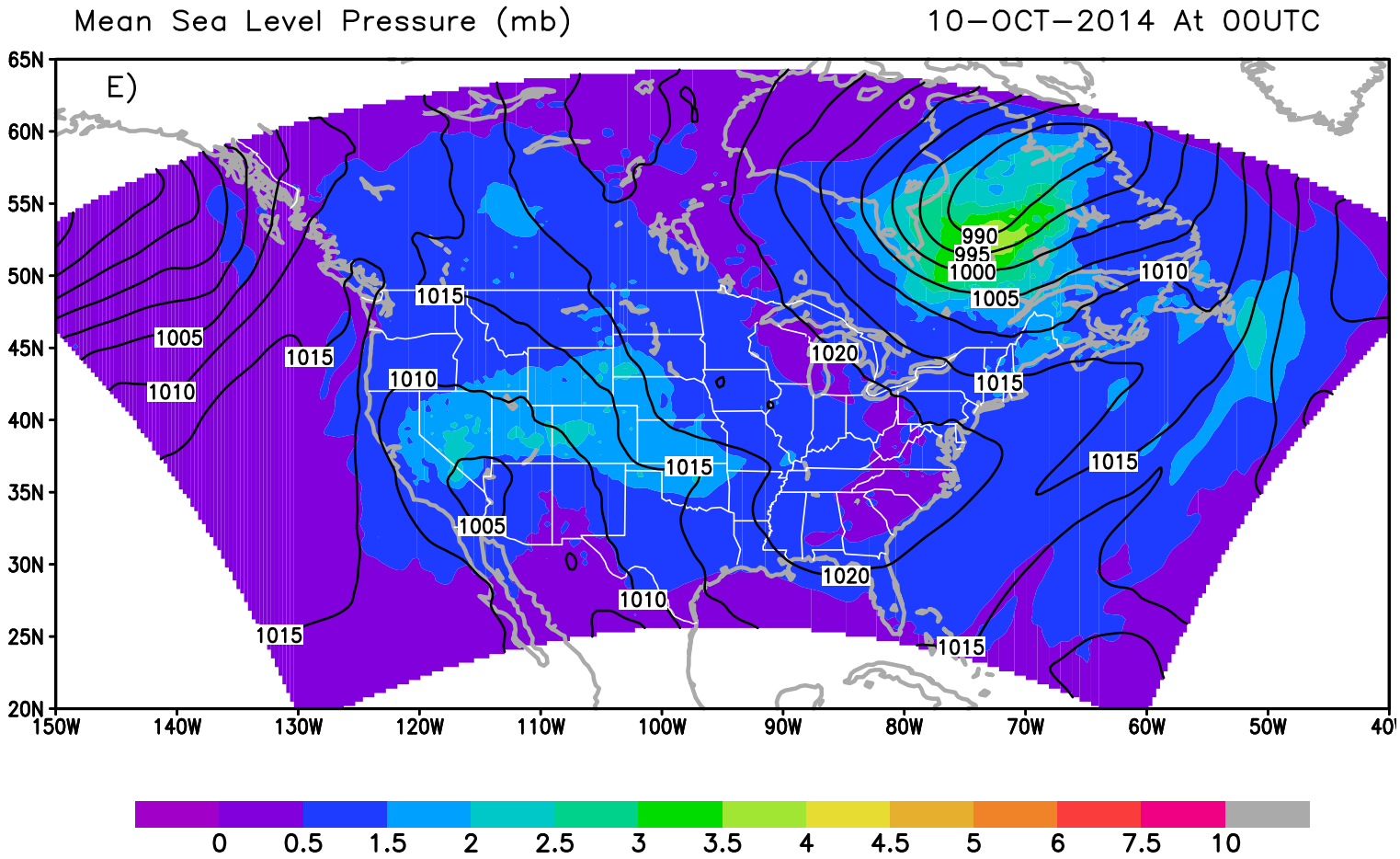
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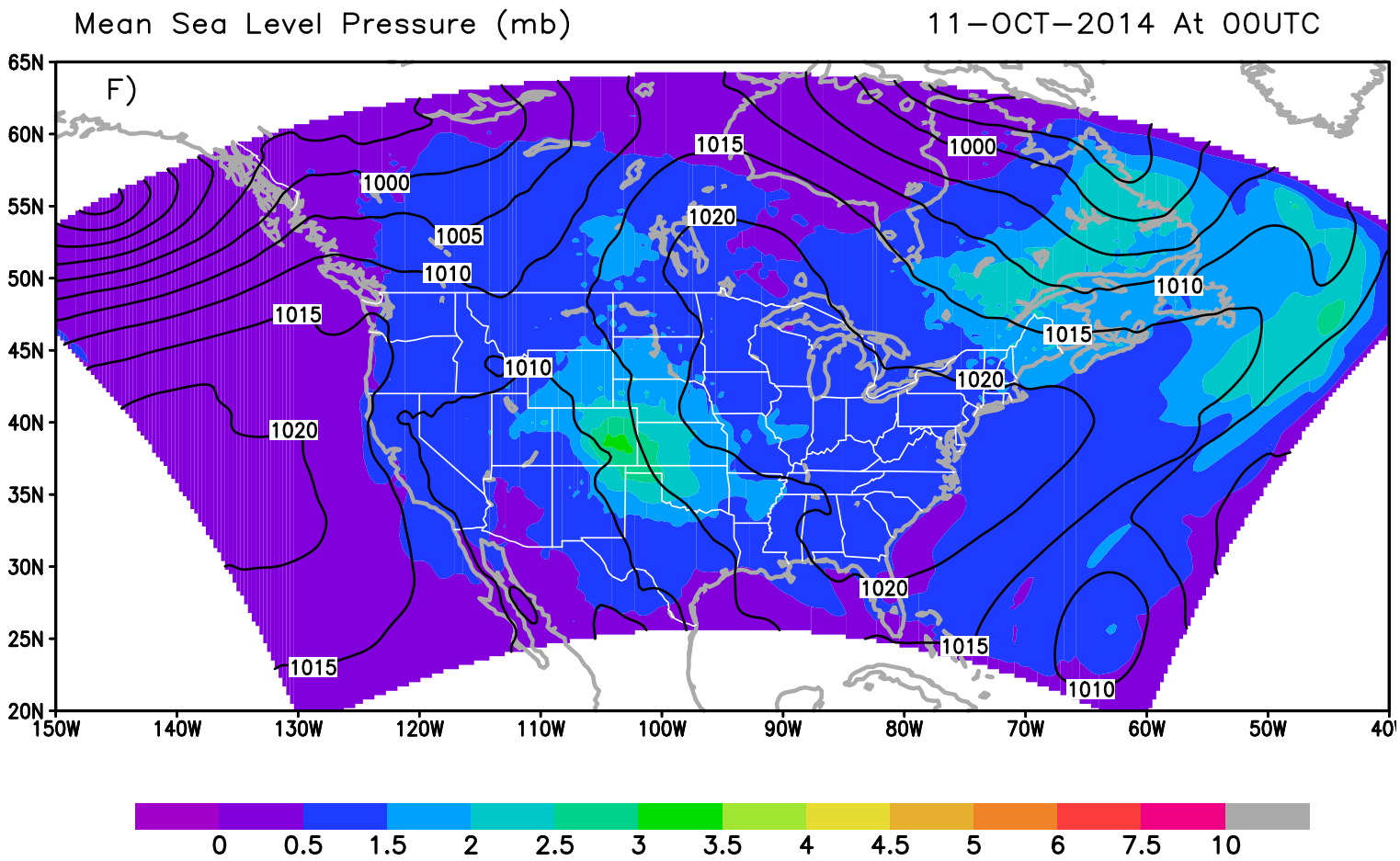
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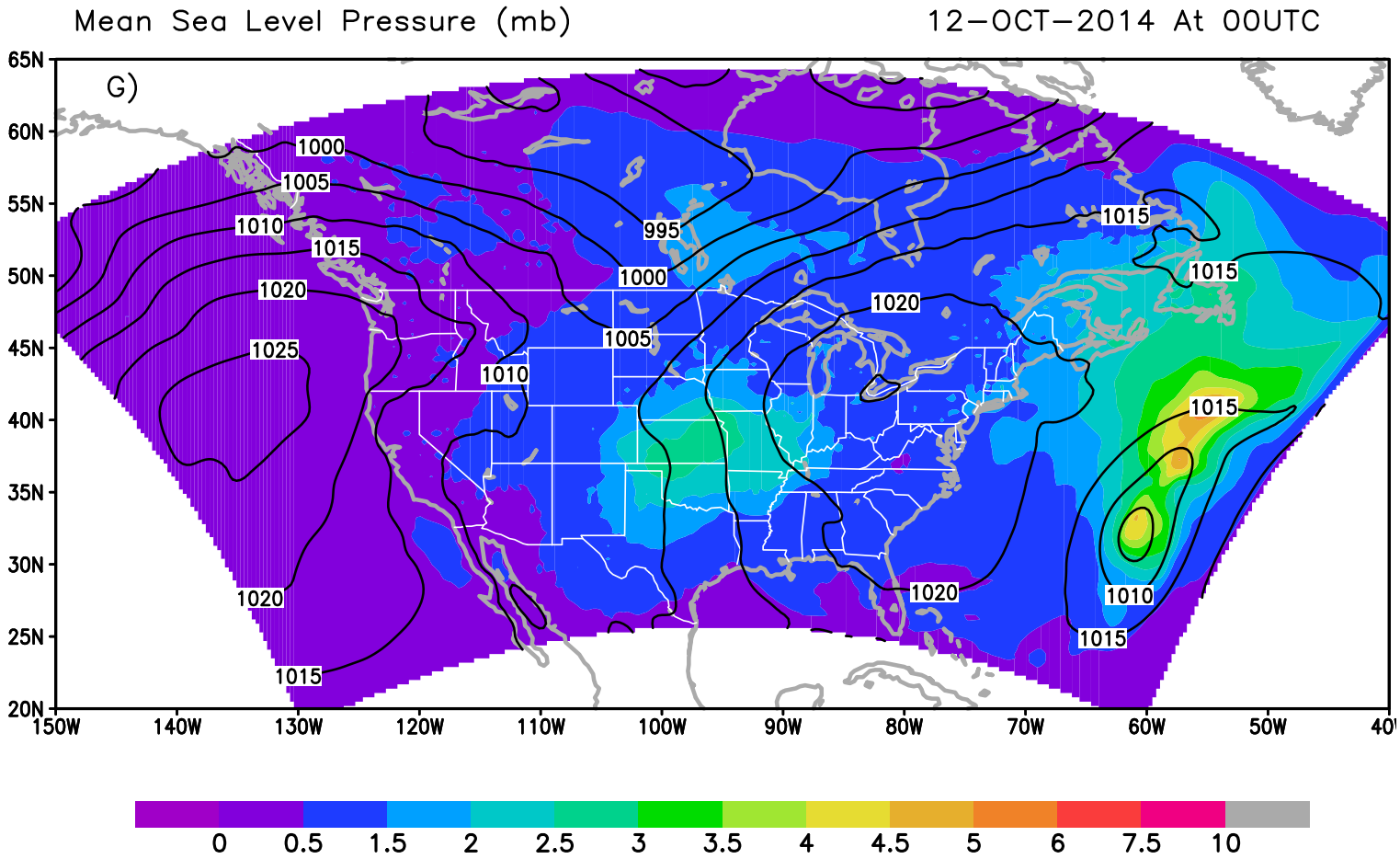
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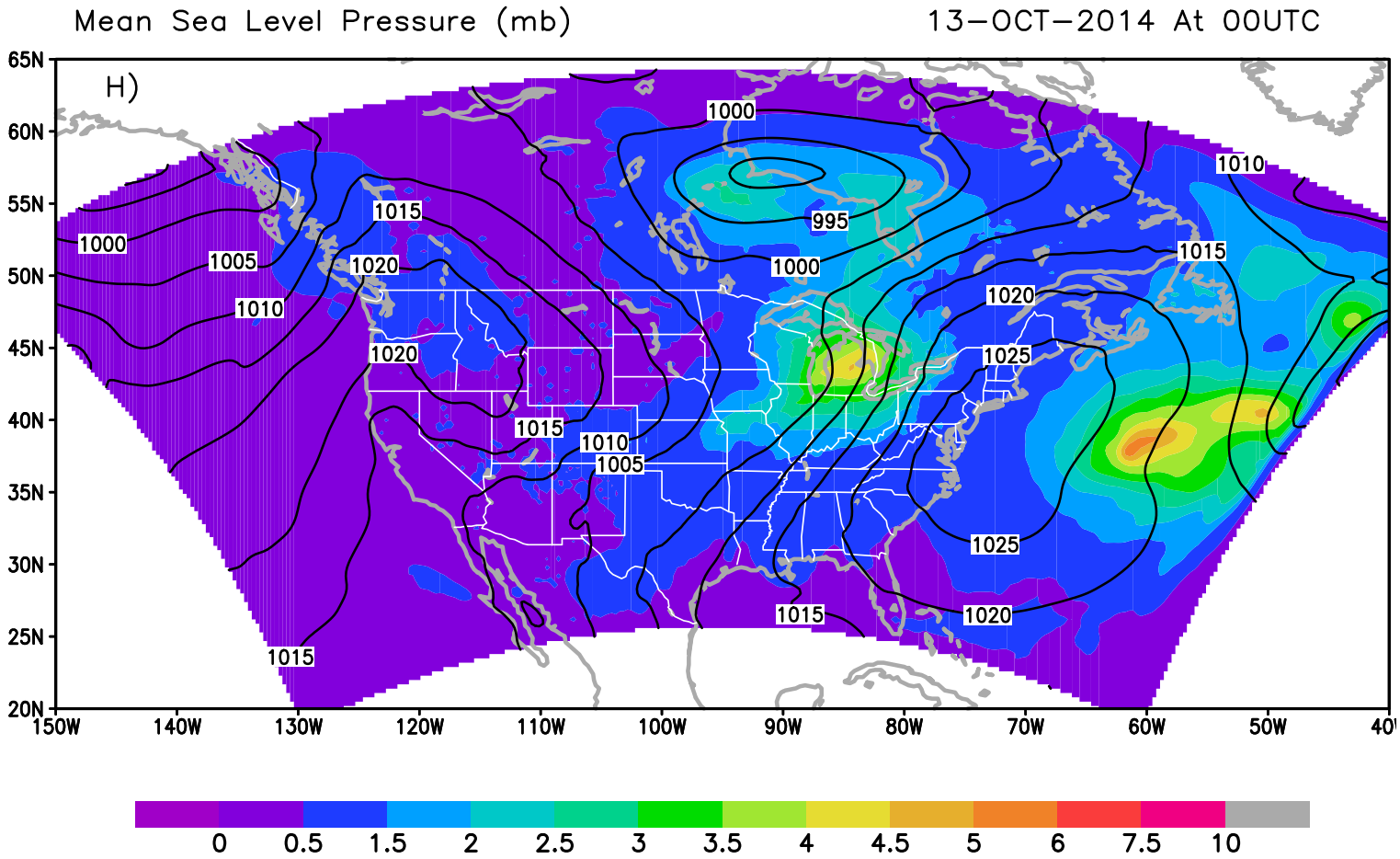
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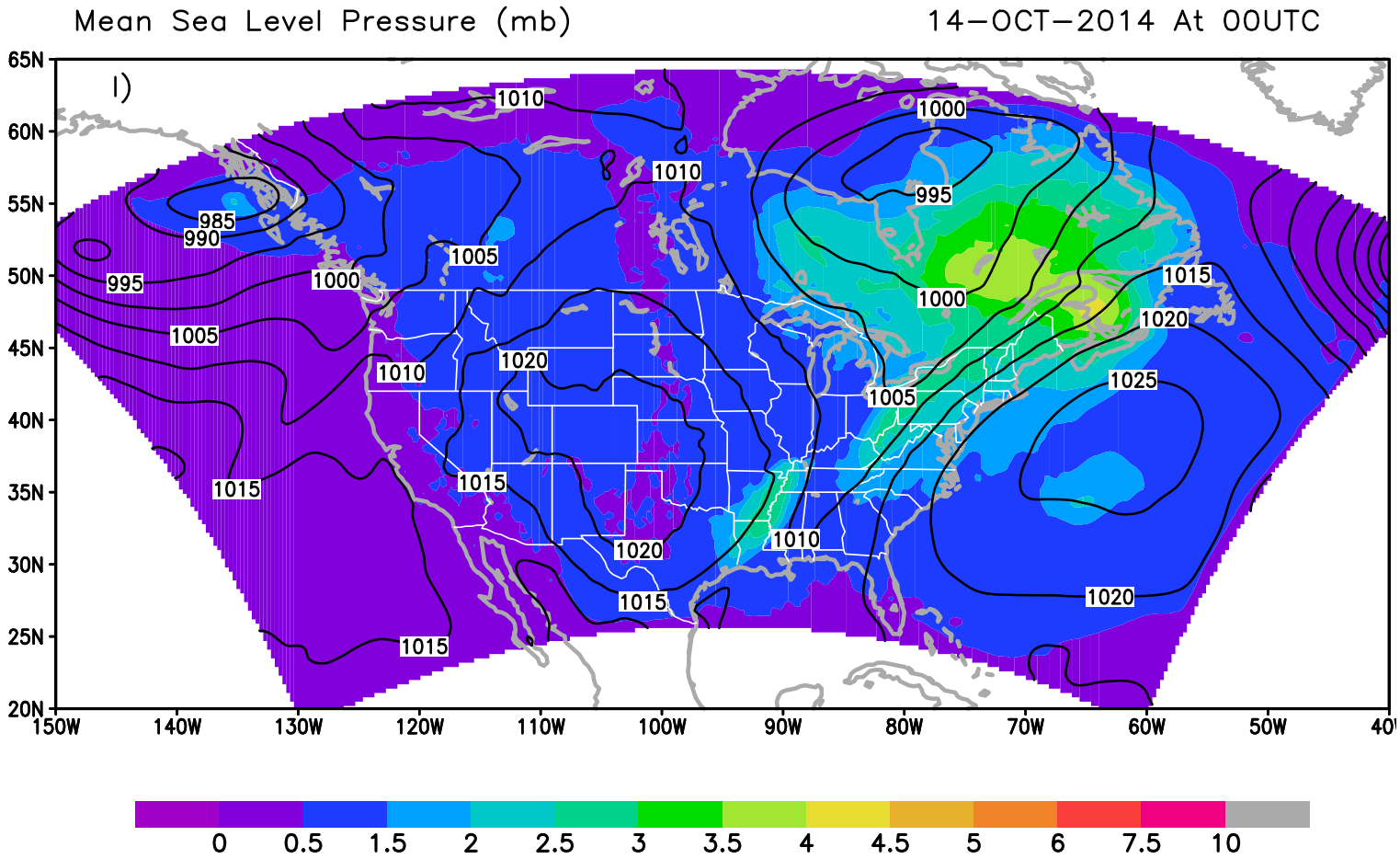
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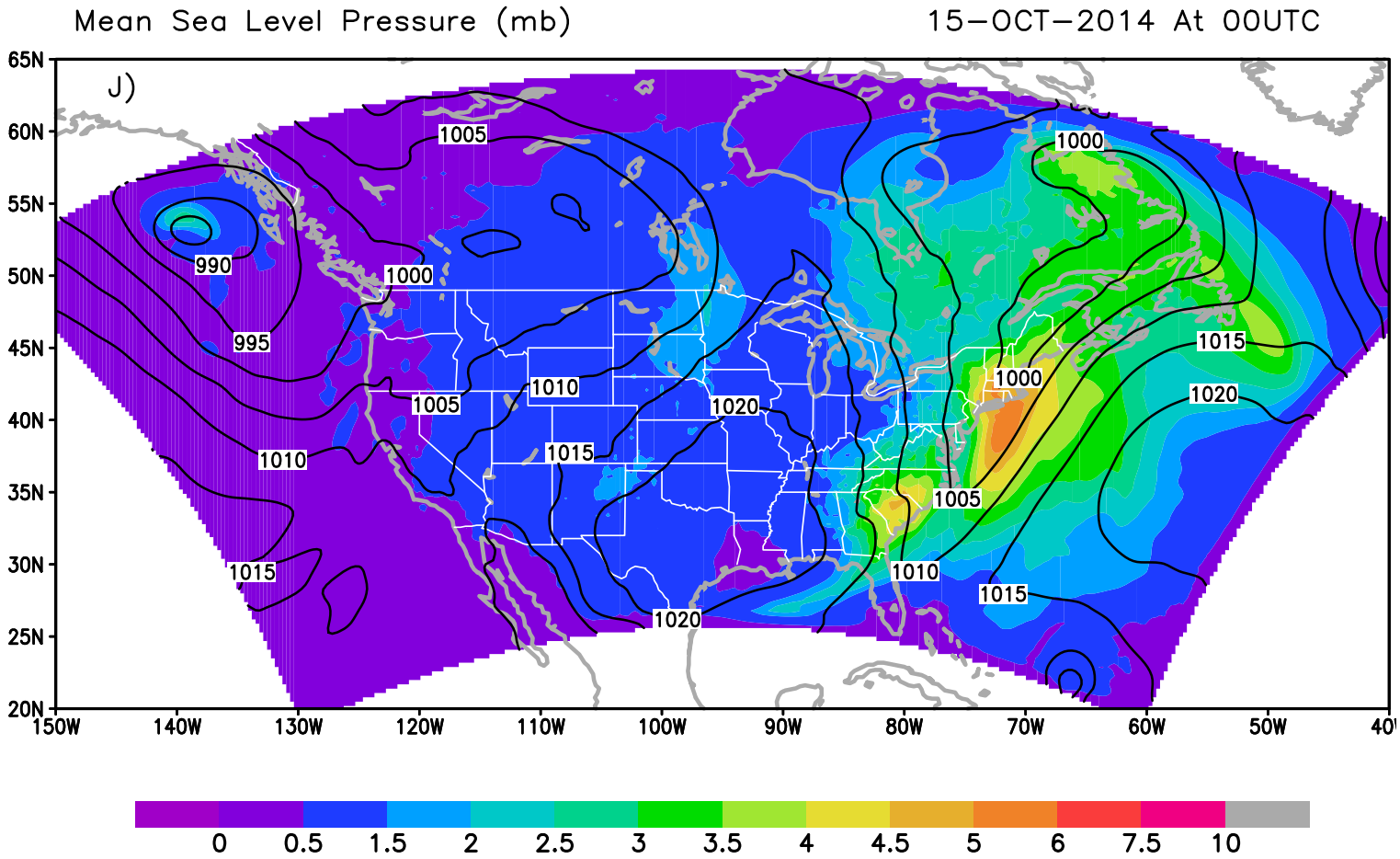
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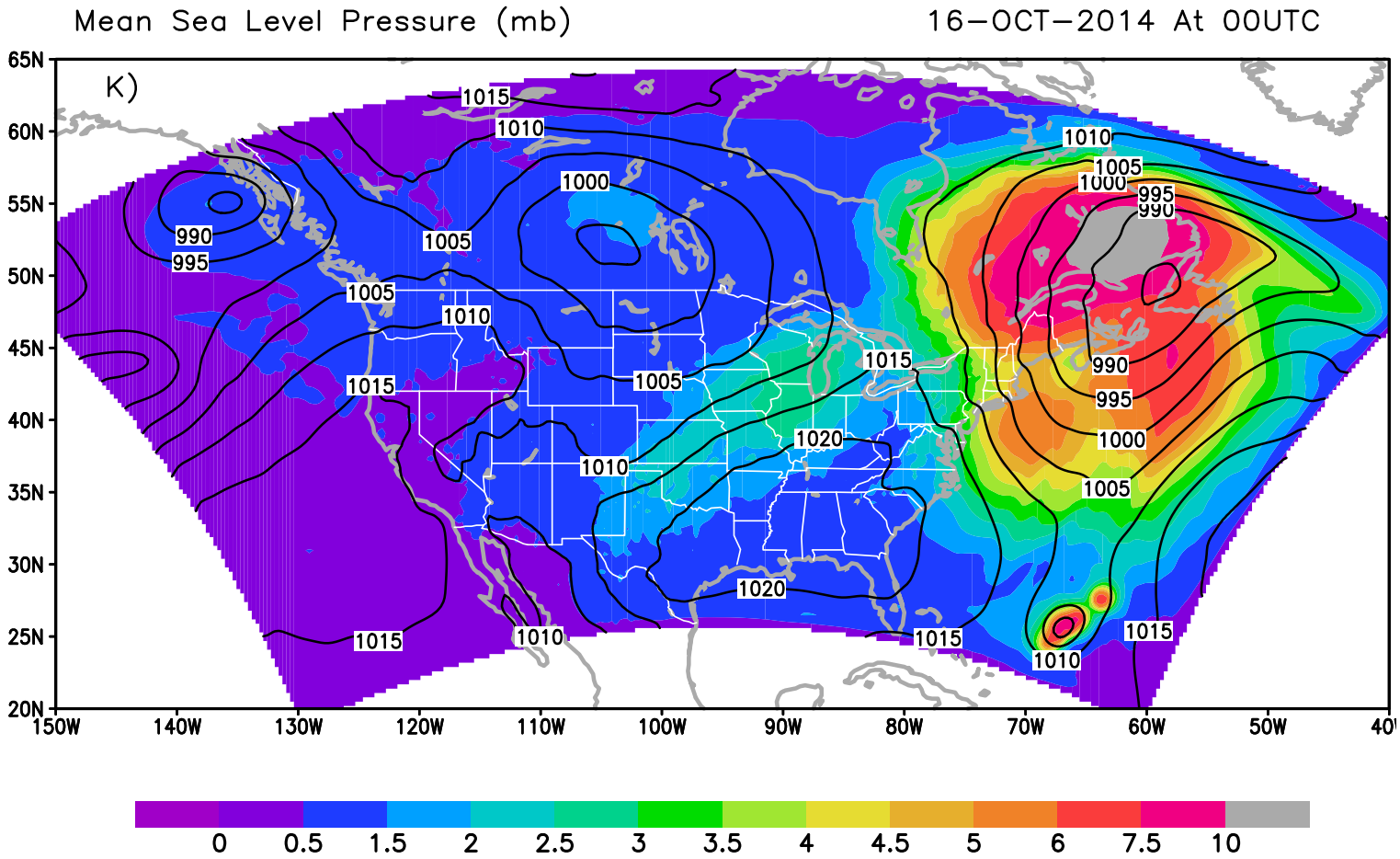
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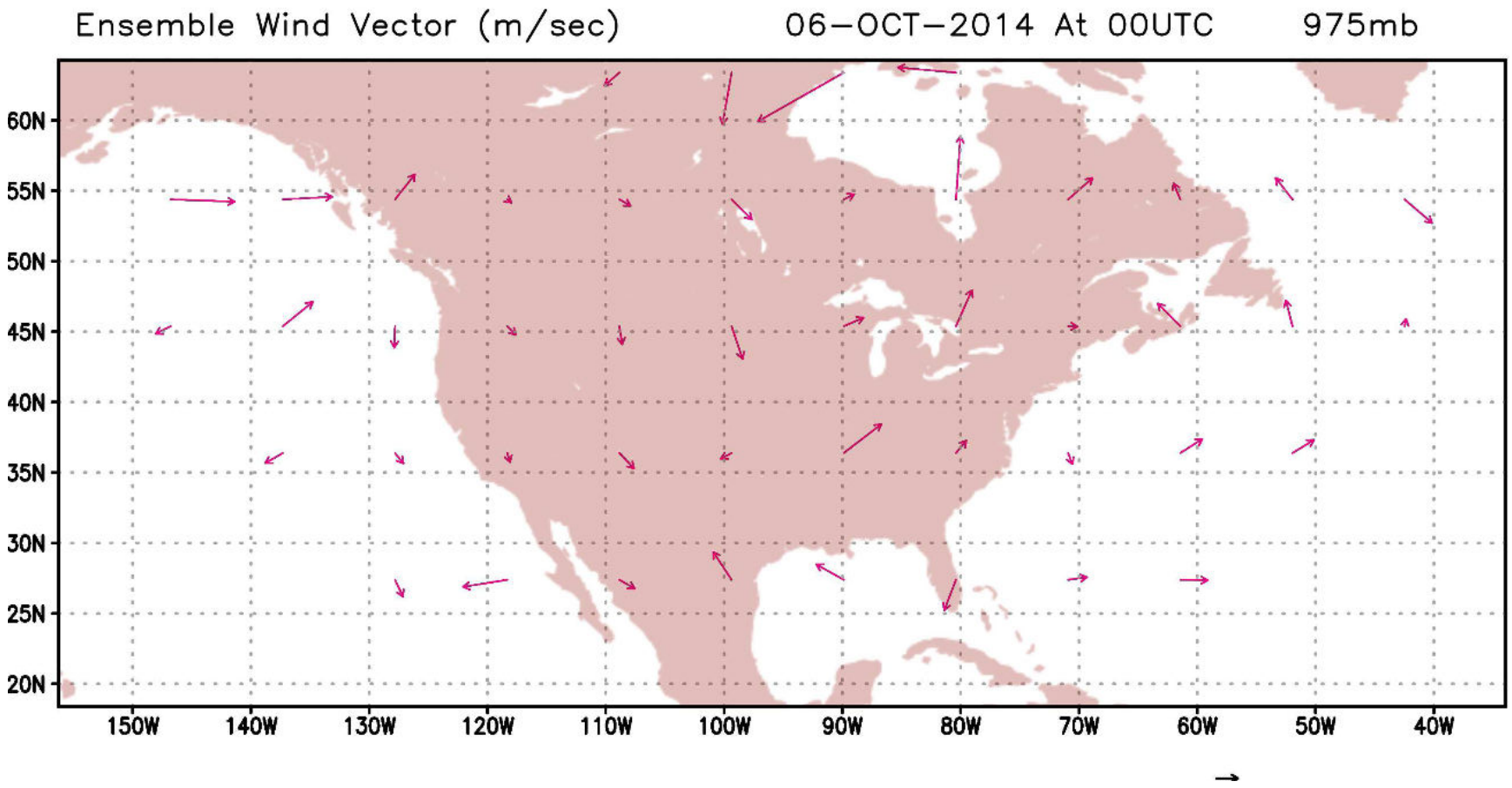
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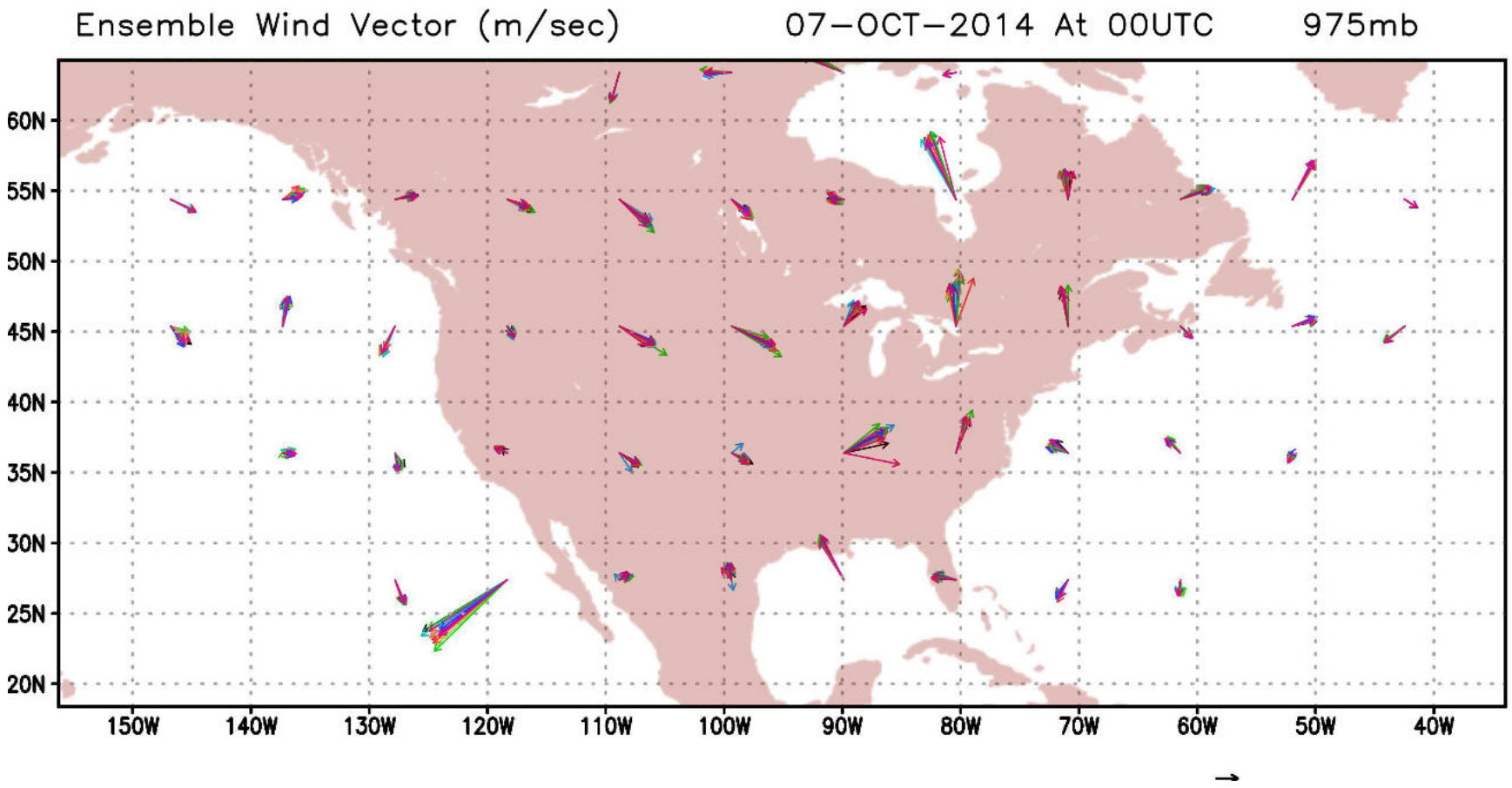
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Wind Variance



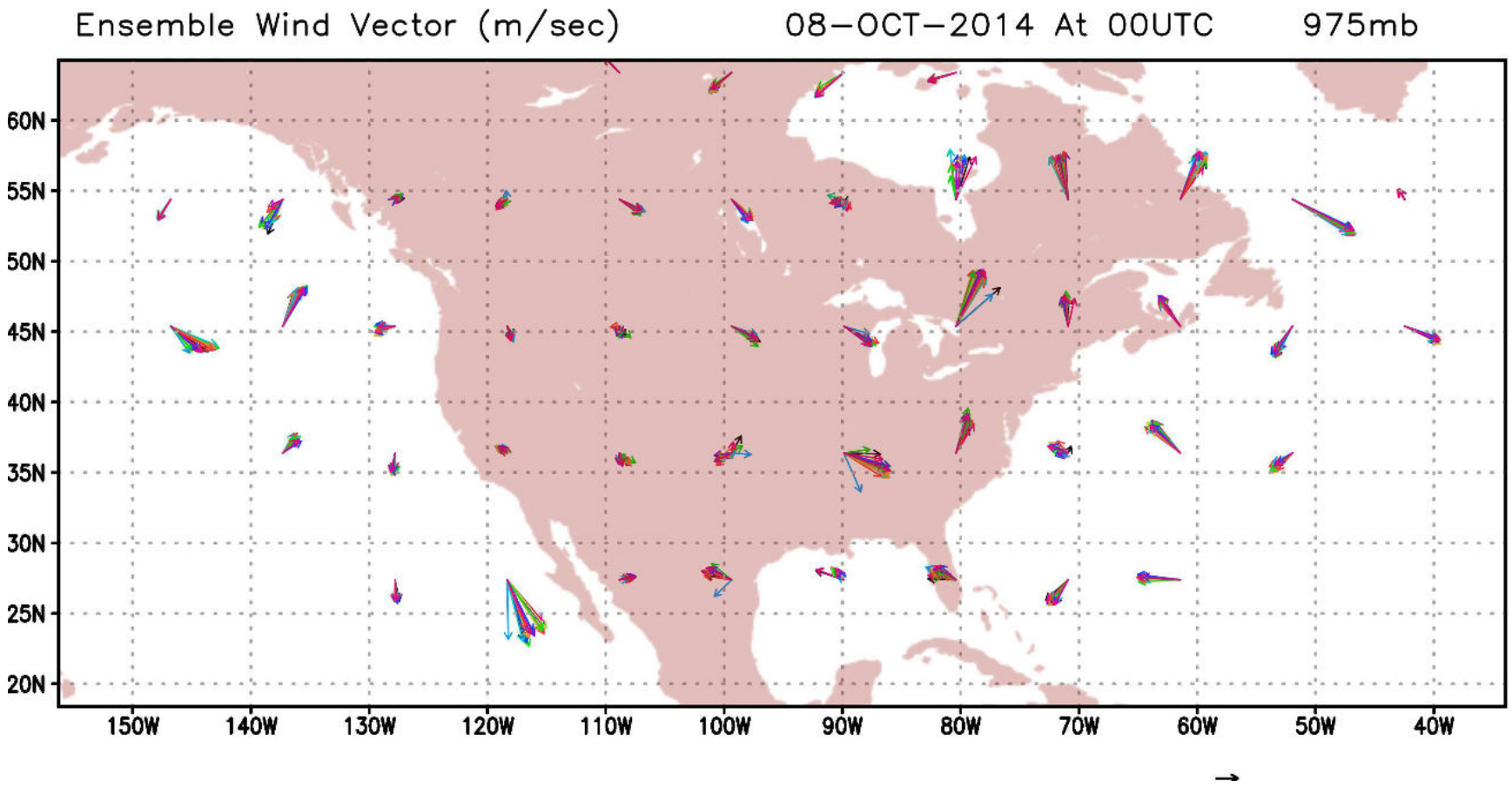
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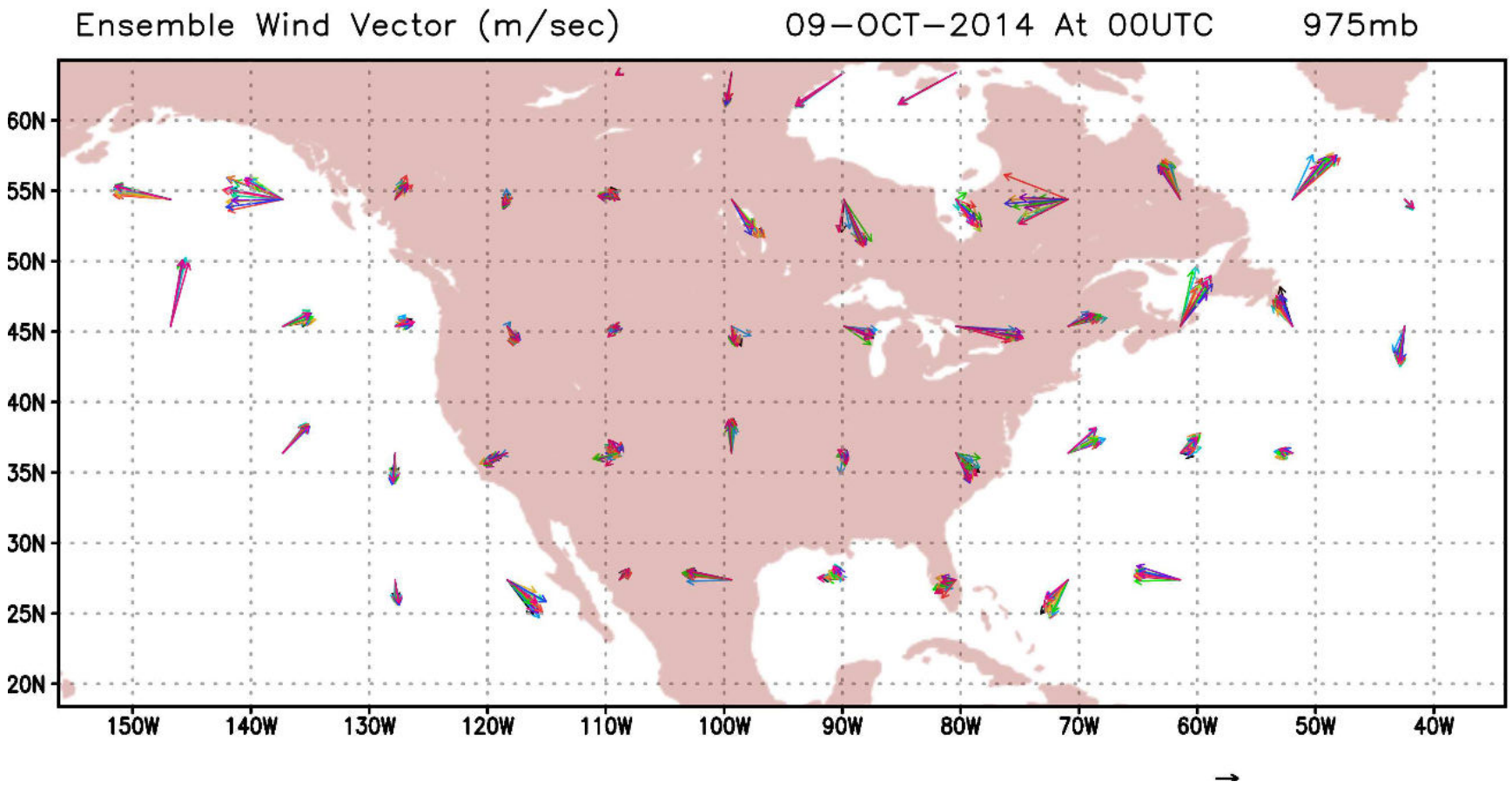
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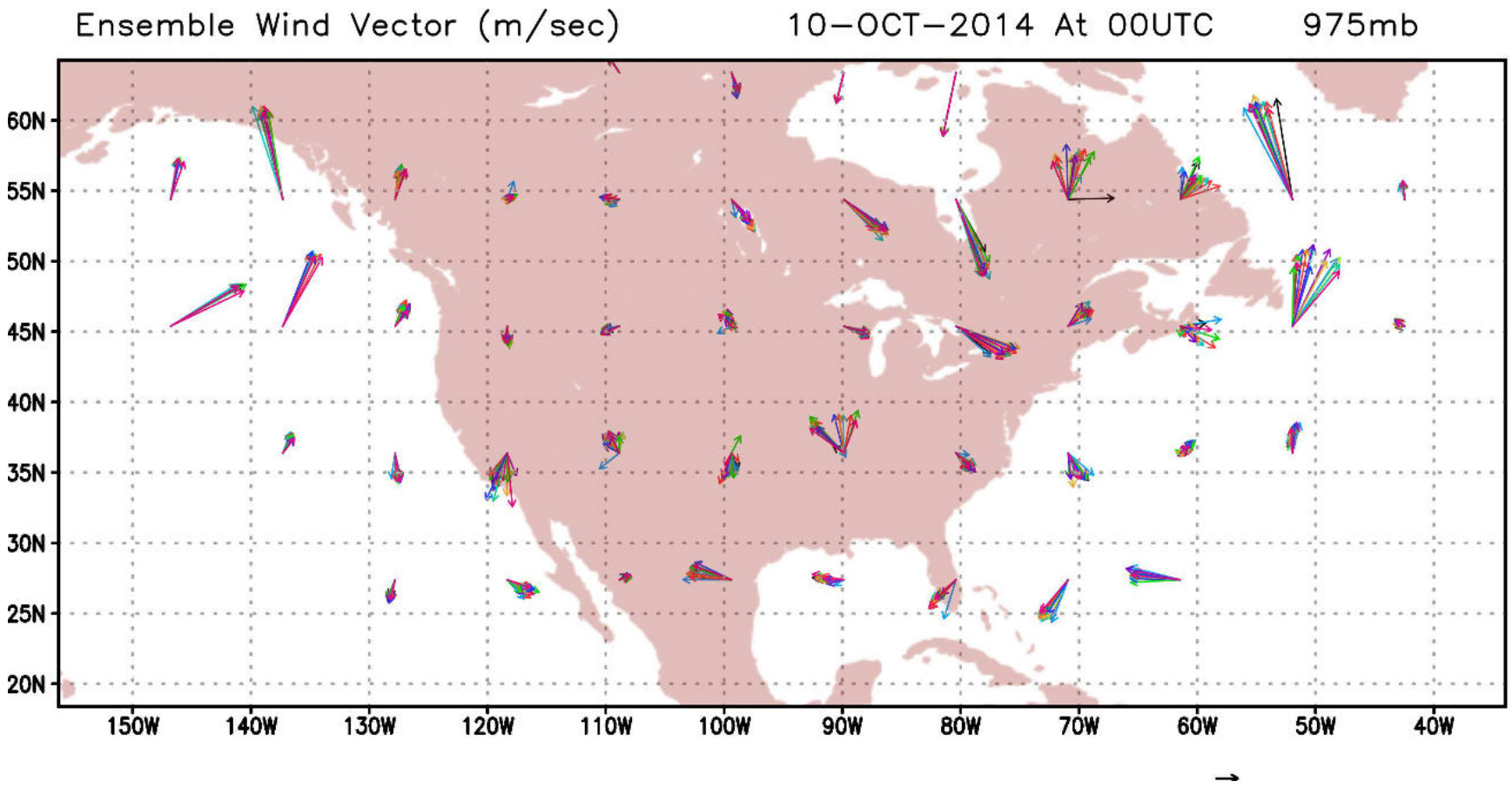
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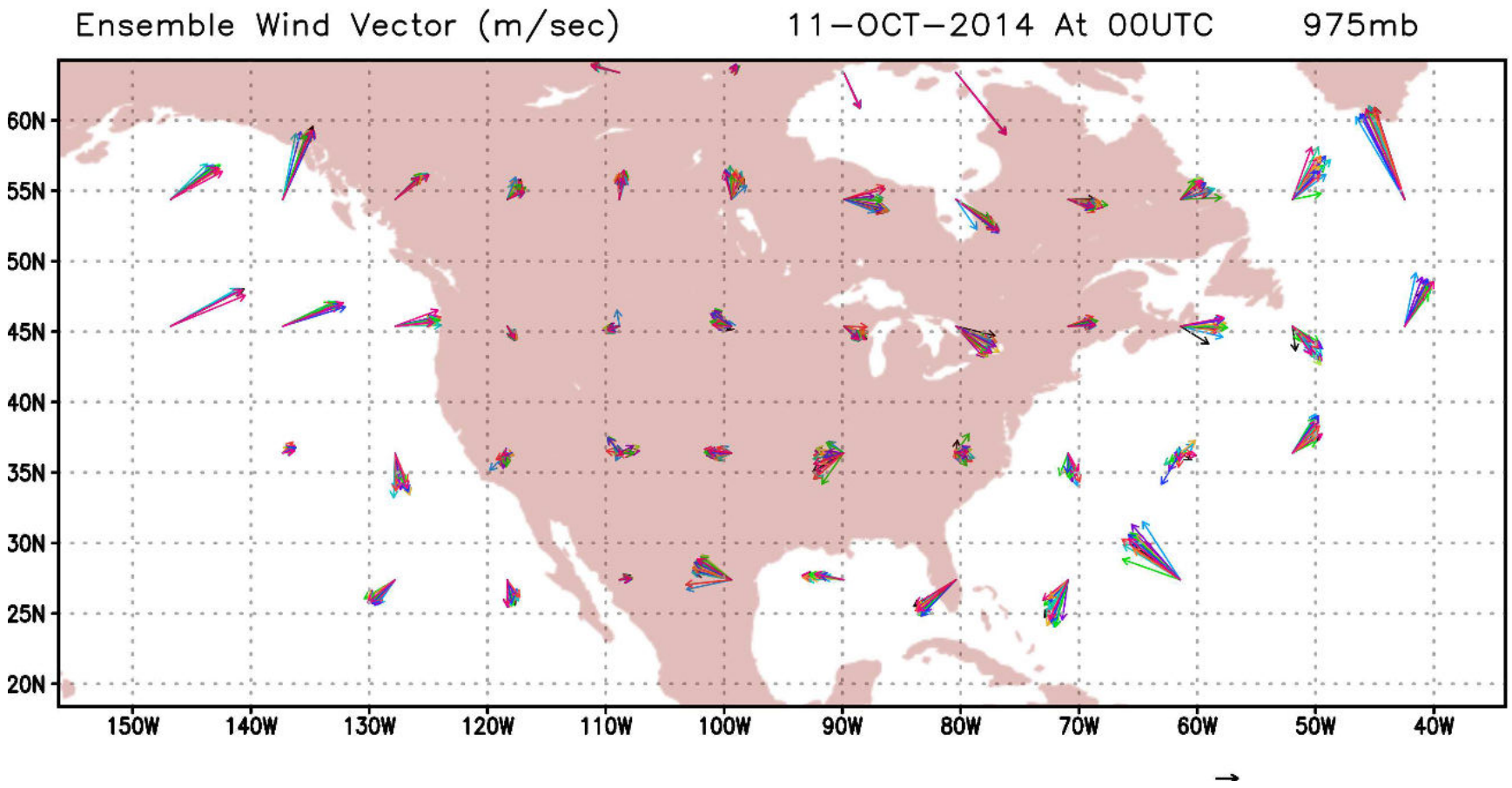
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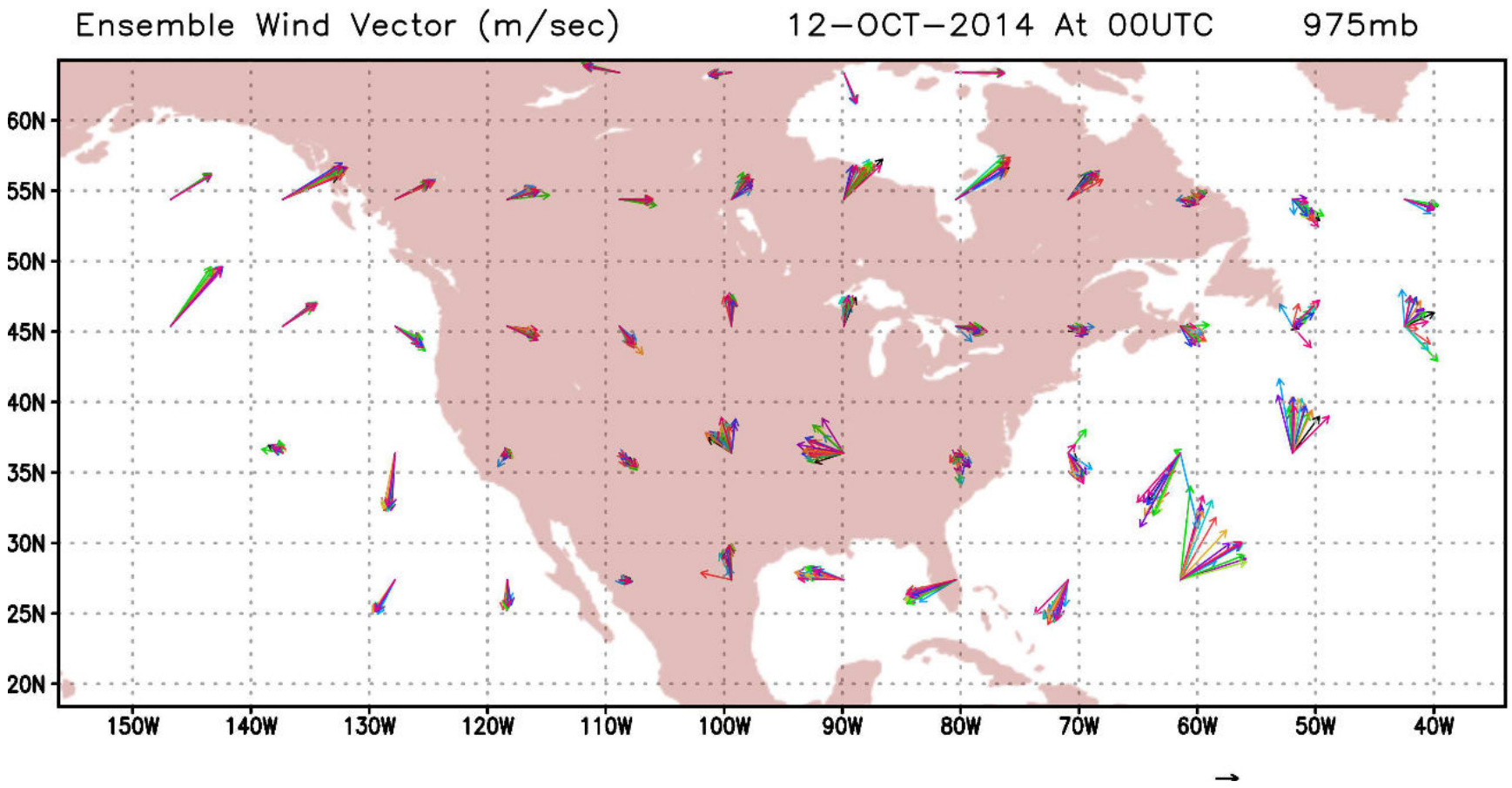
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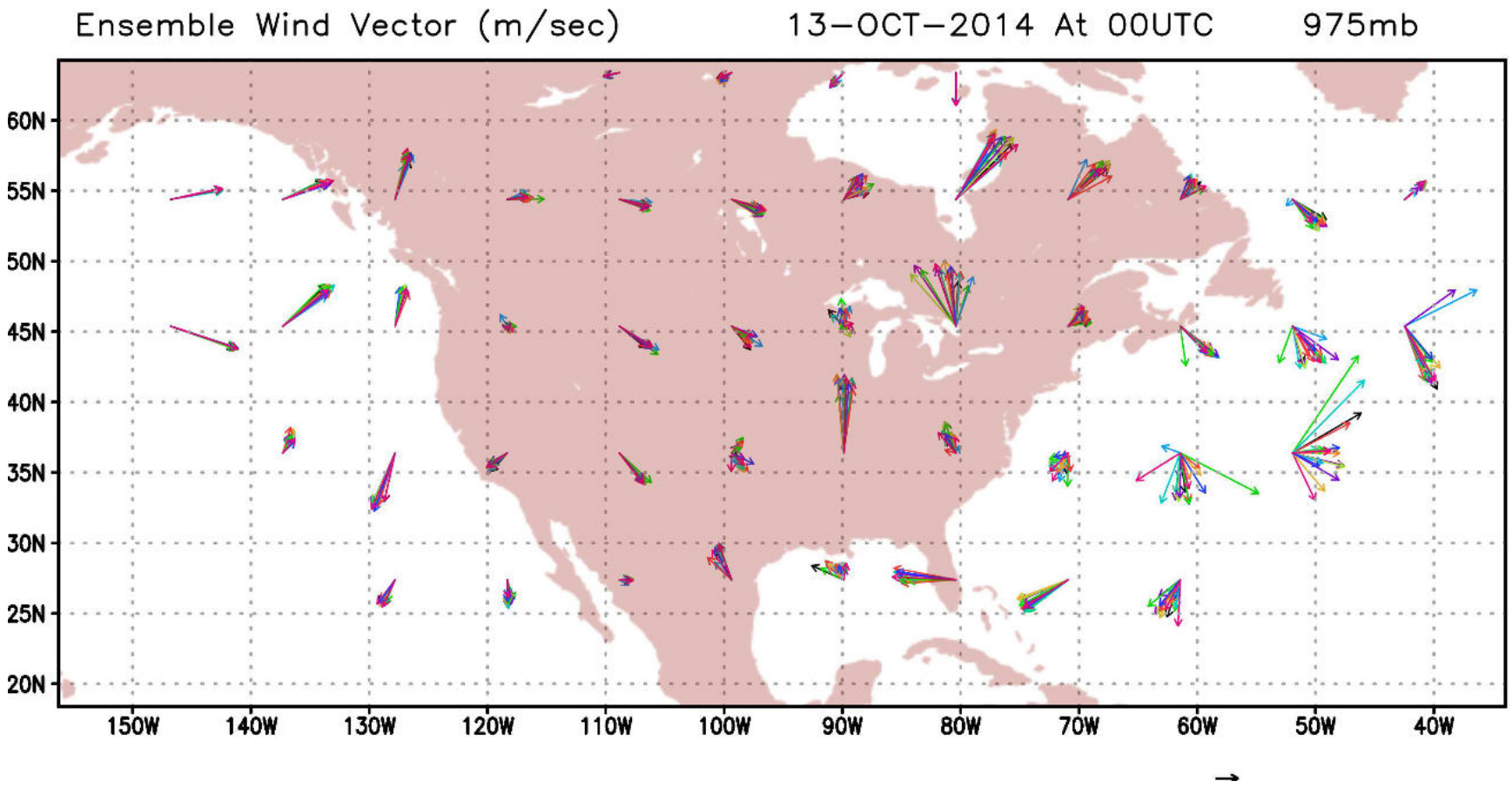
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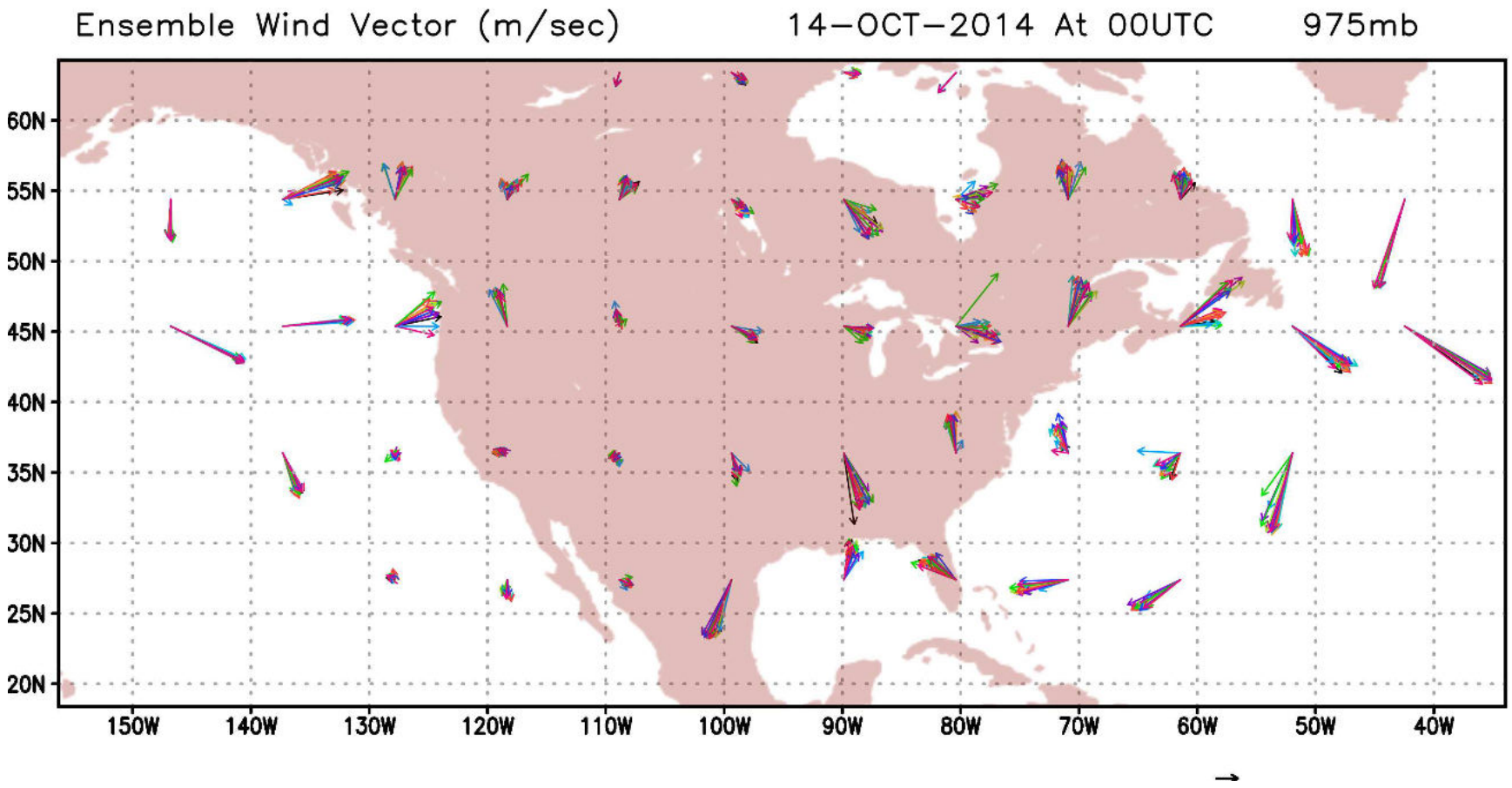
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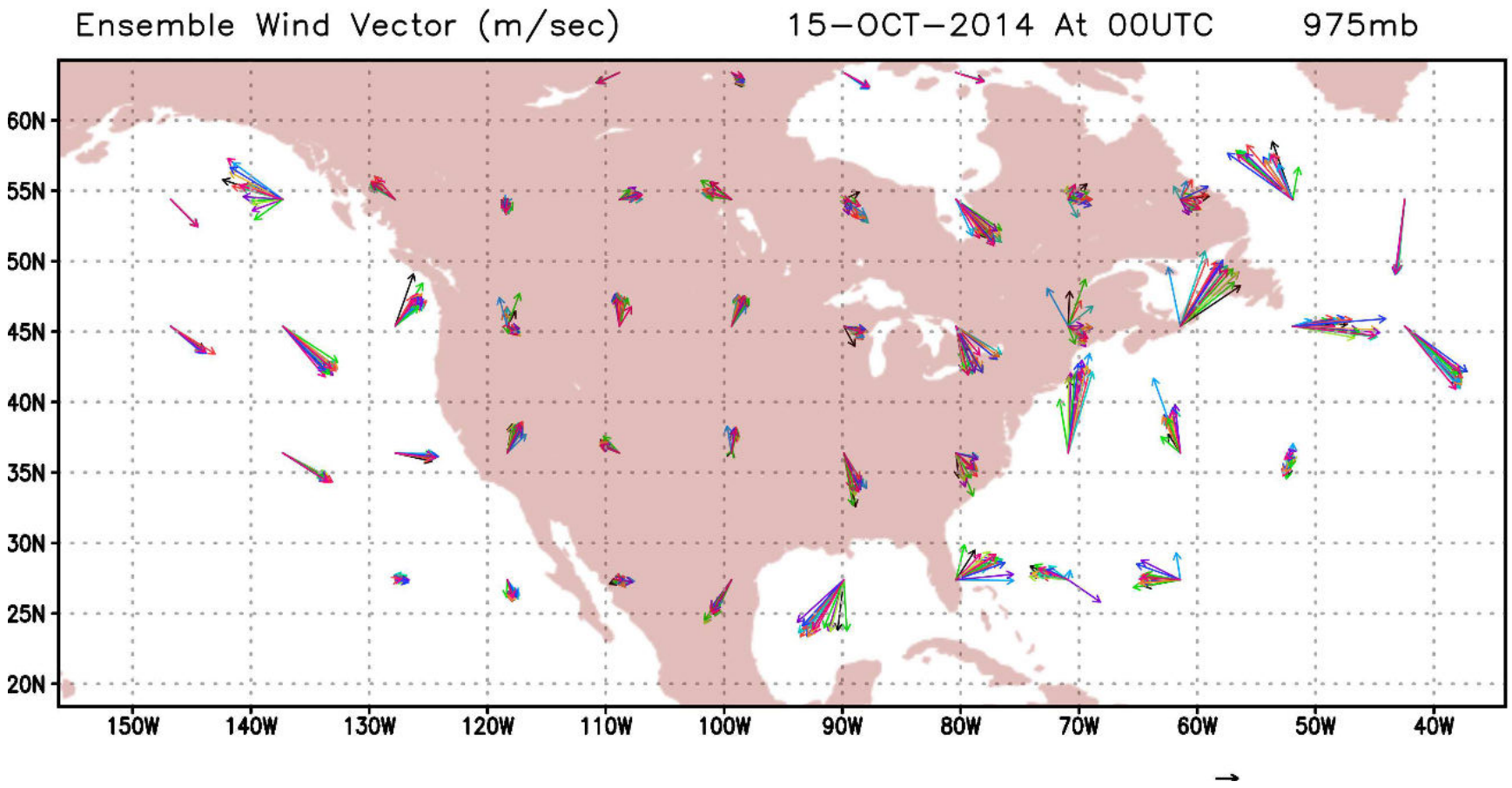
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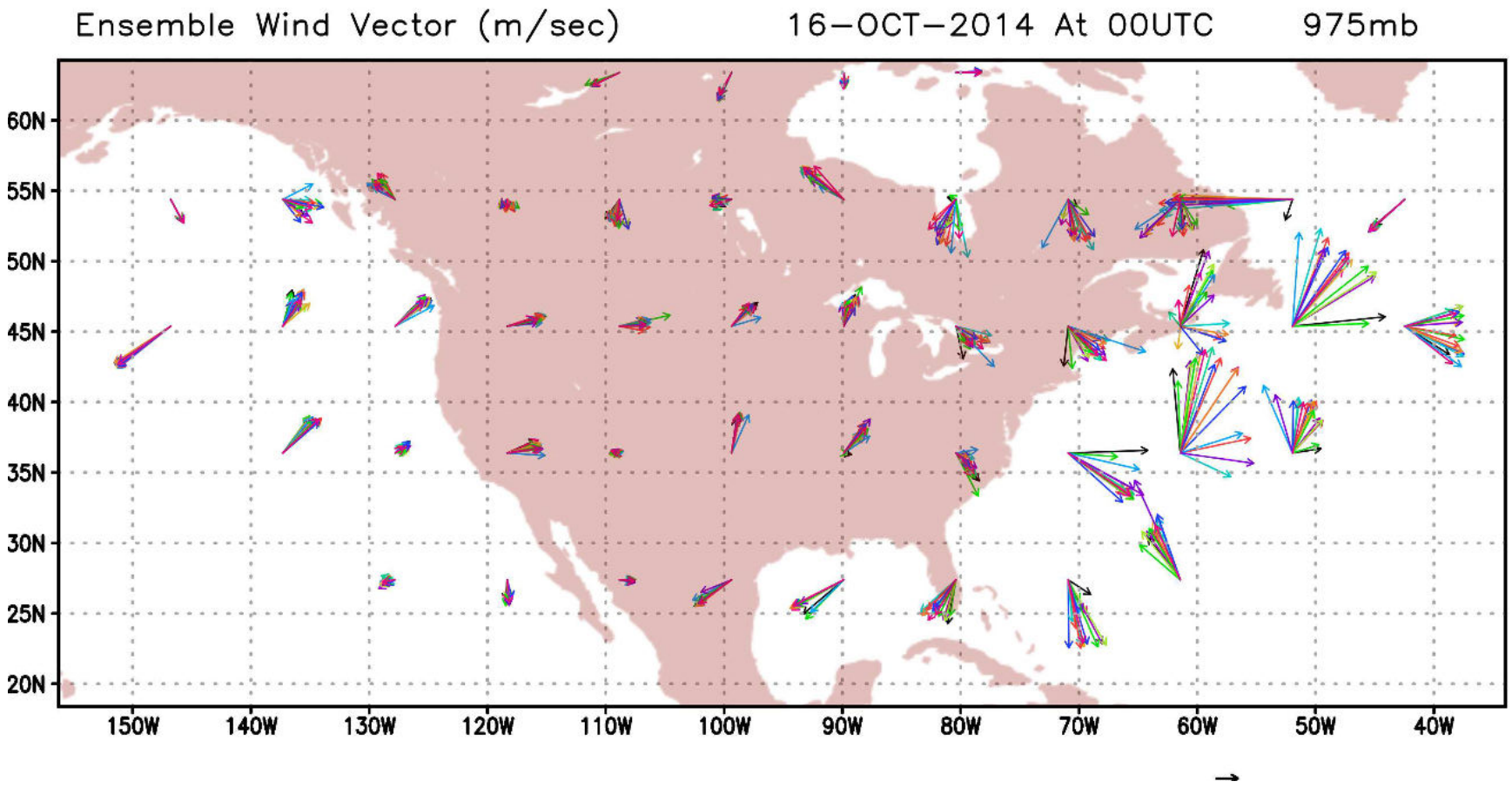
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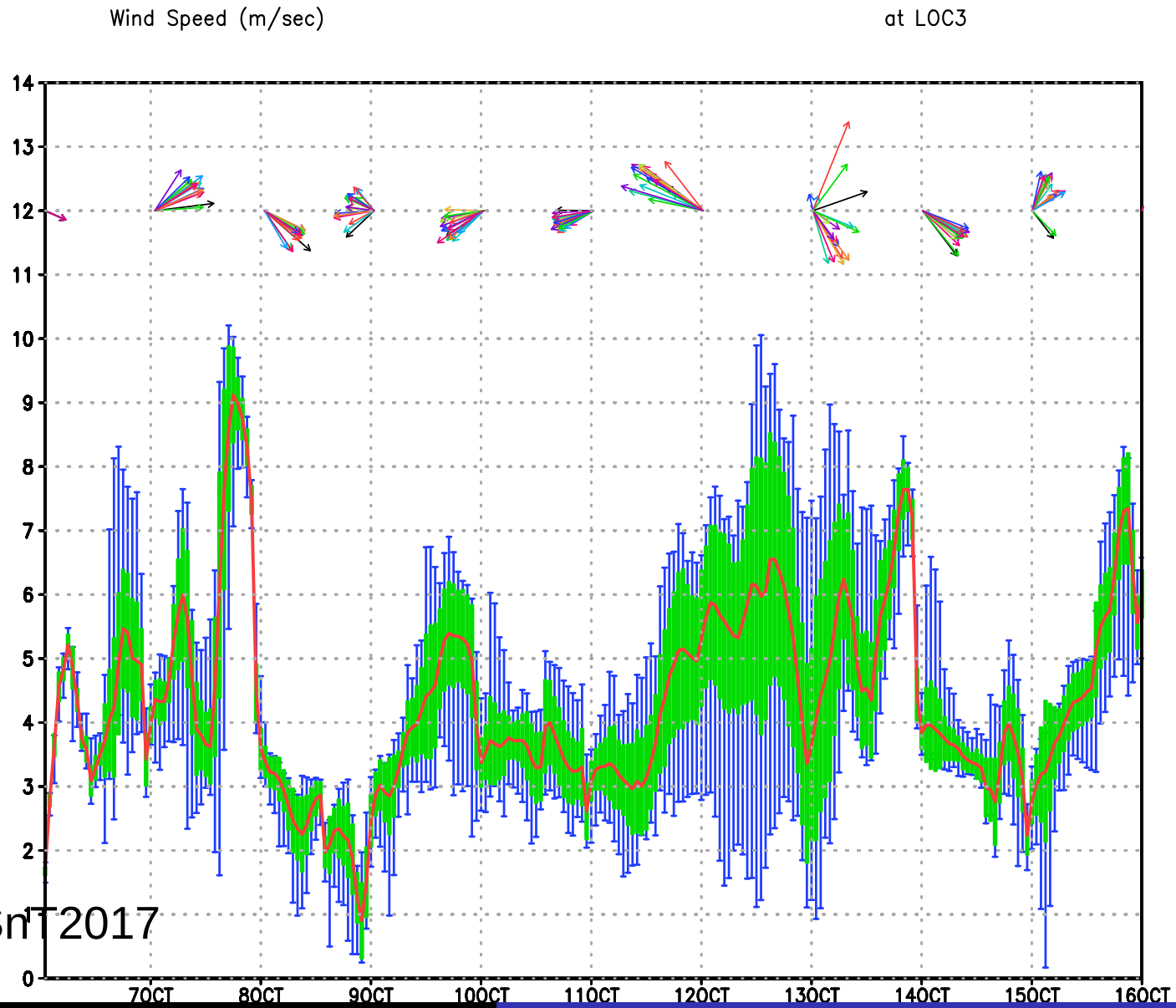
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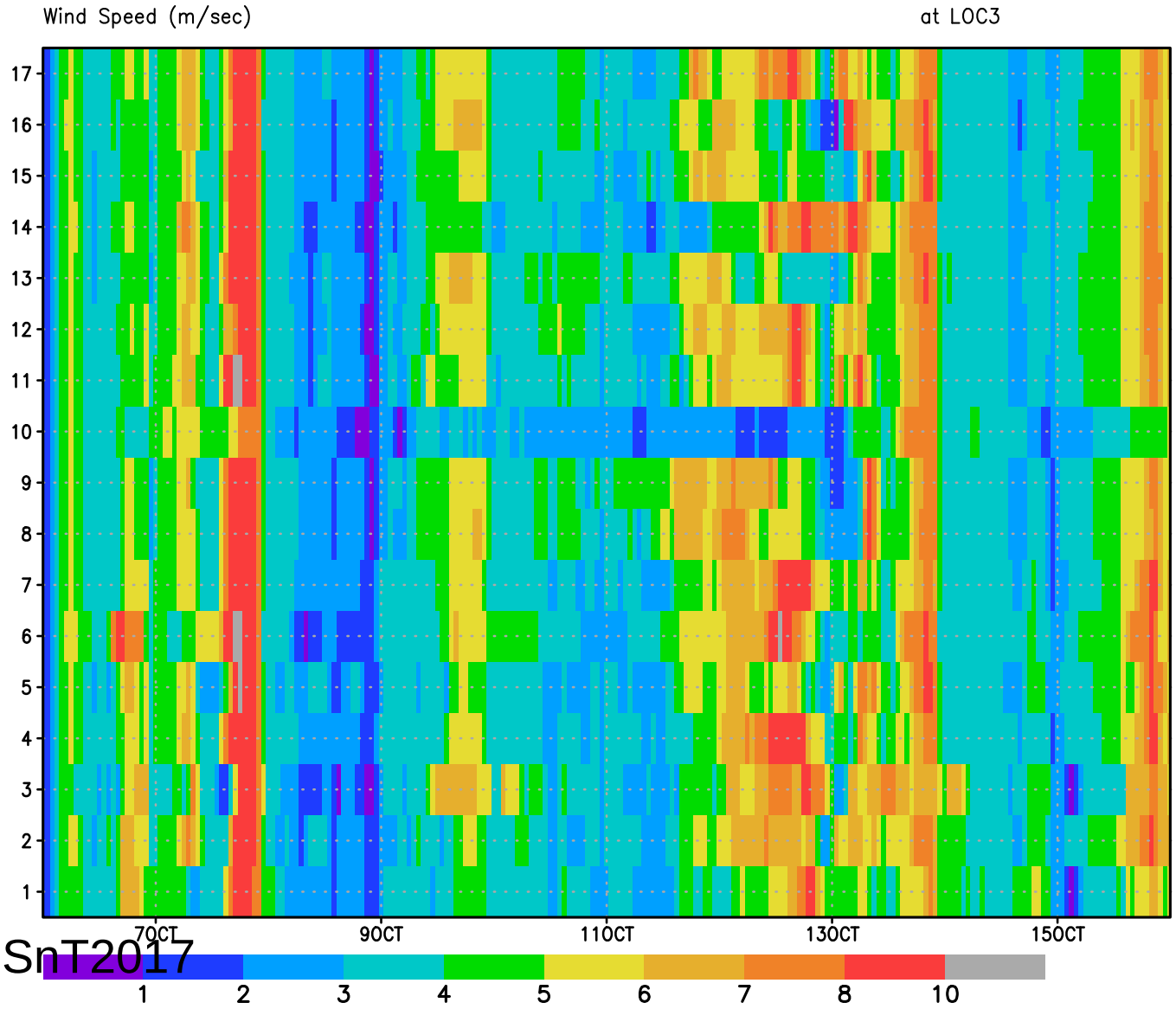
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Whisker Diagrams (Wind)



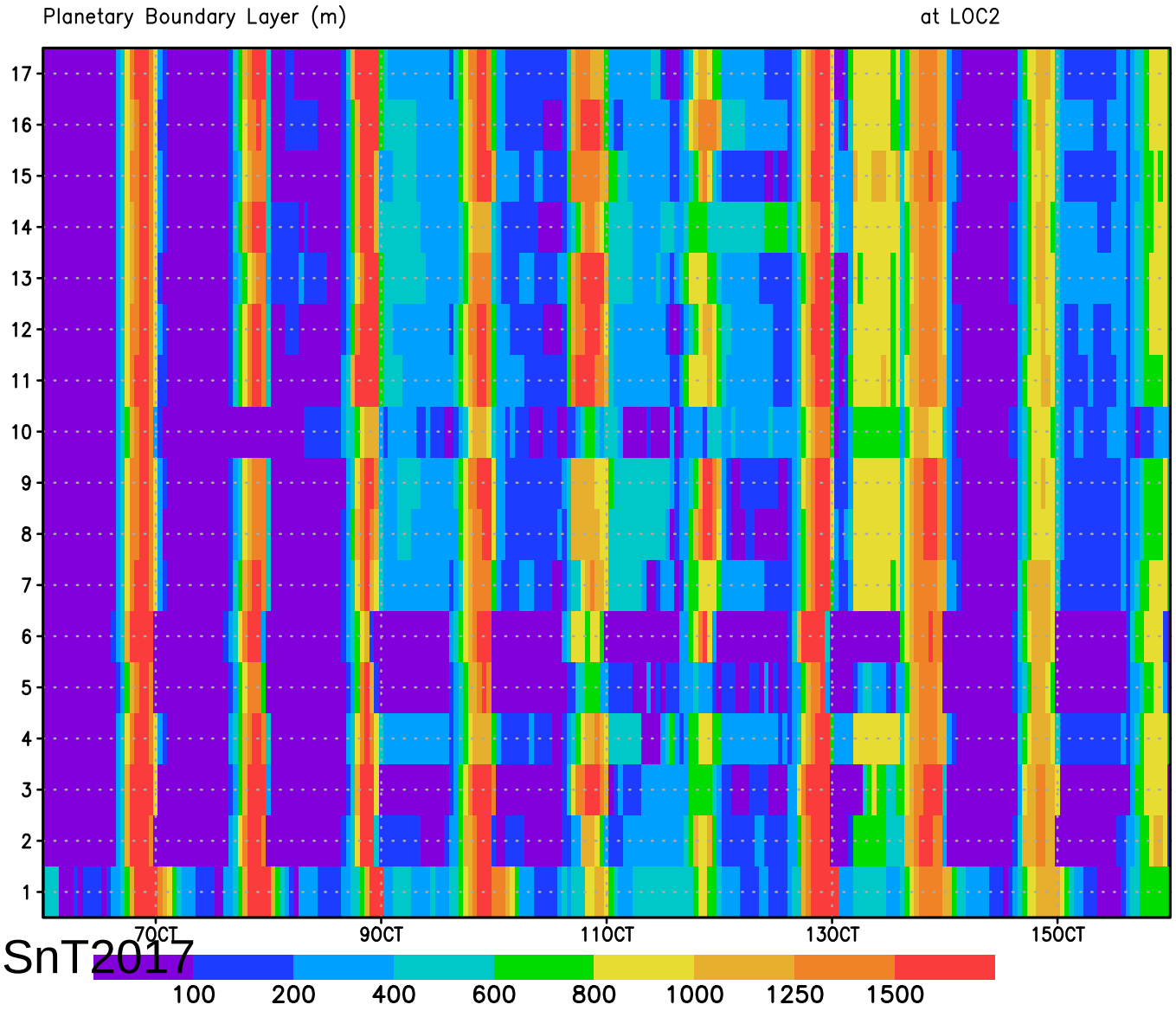
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Shaded Boxes(Wind)



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Shaded Boxes(PBL)



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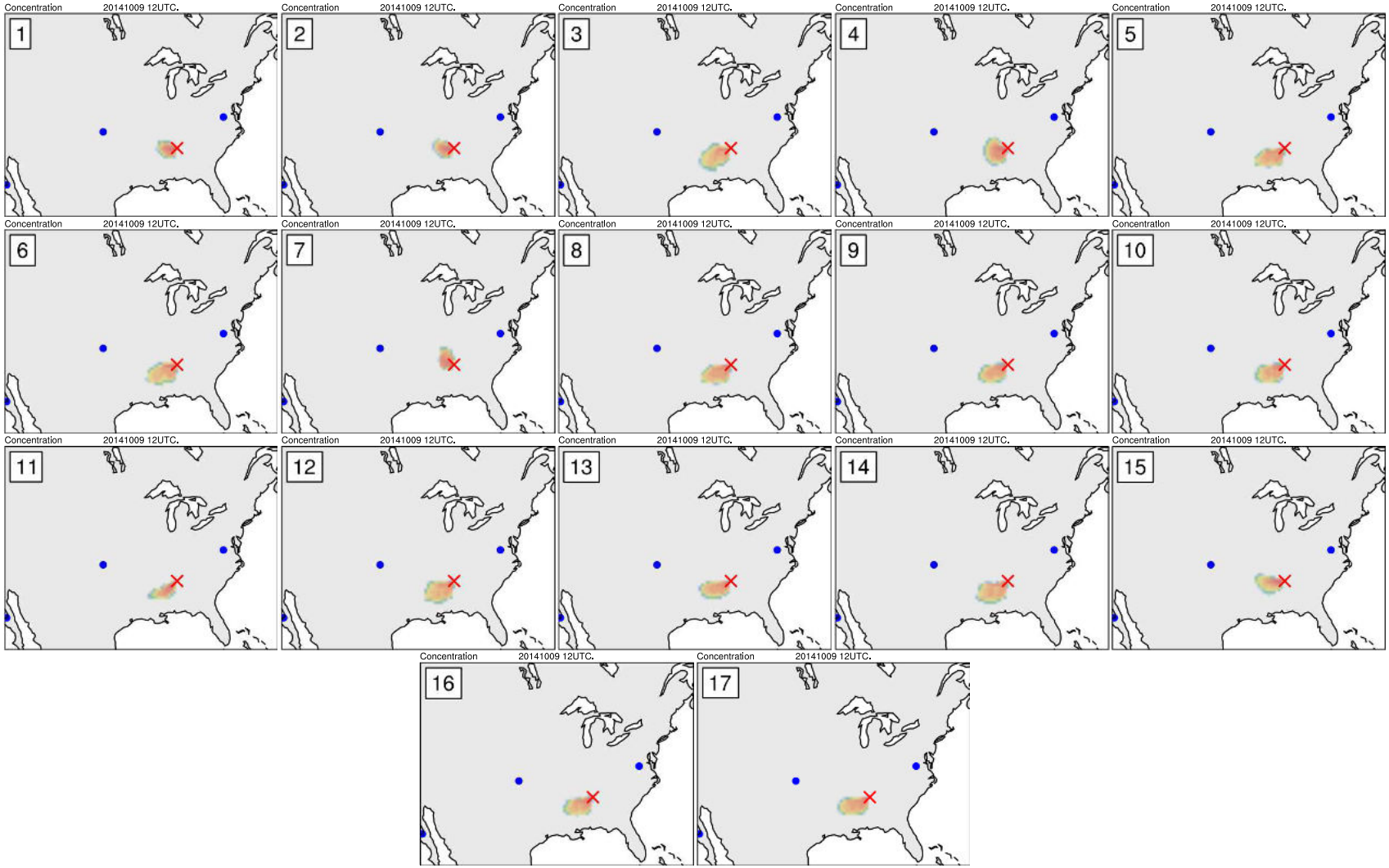
Outline

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Plume Ensemble Members

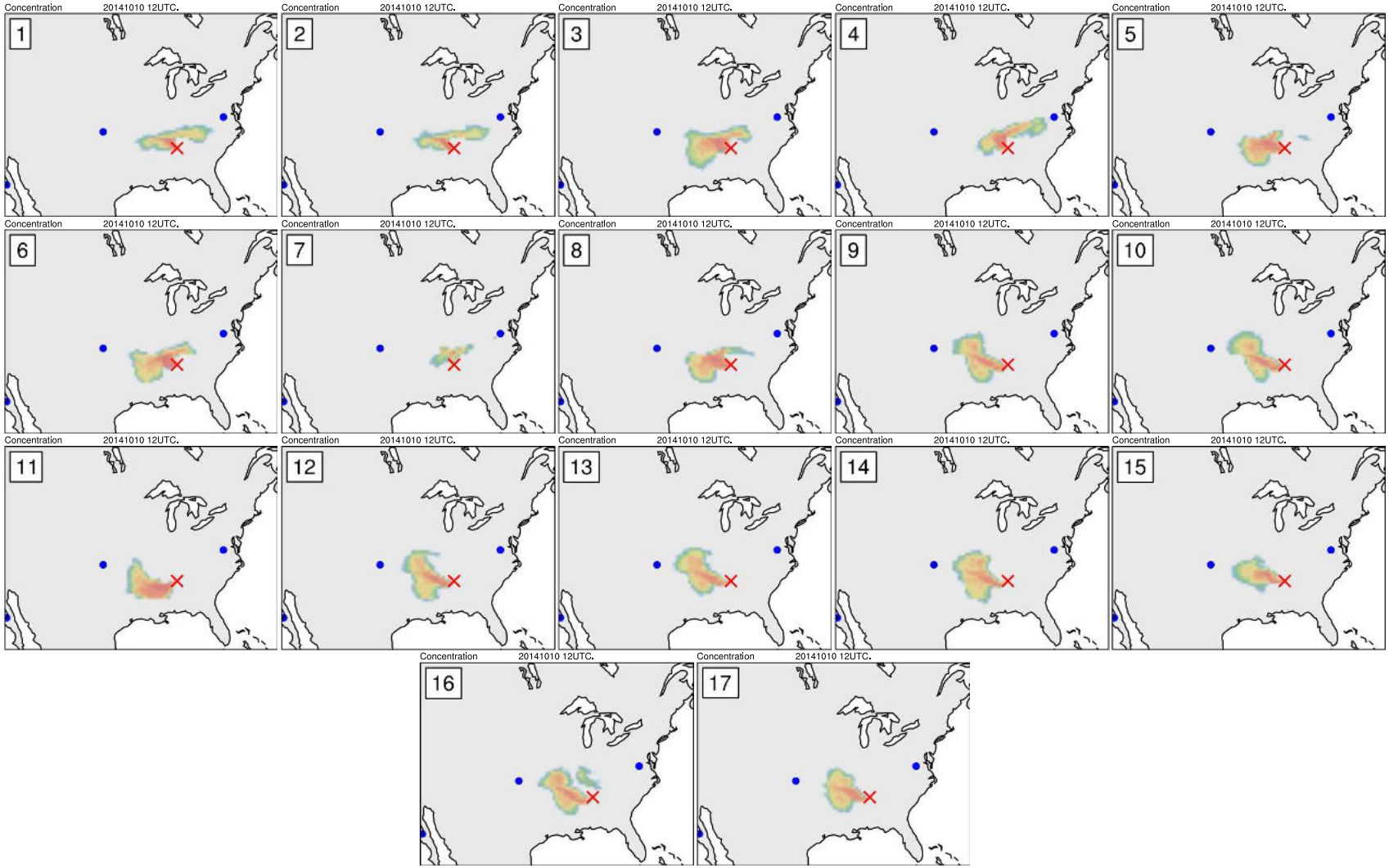
Releases from LOC4: on 9 Oct. 2014



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Plume Ensemble Members

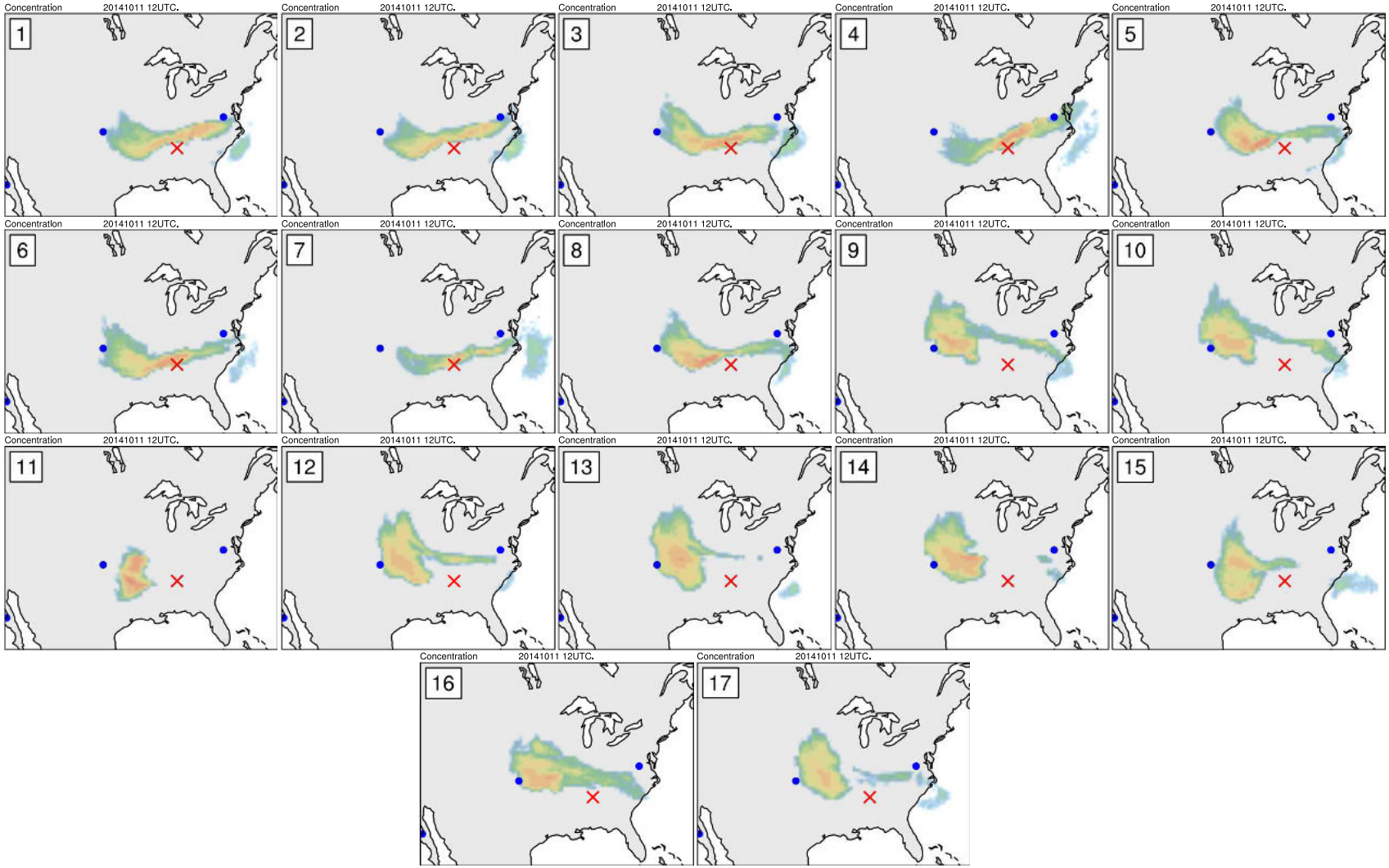
Releases from LOC4: on 10 Oct. 2014



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Plume Ensemble Members

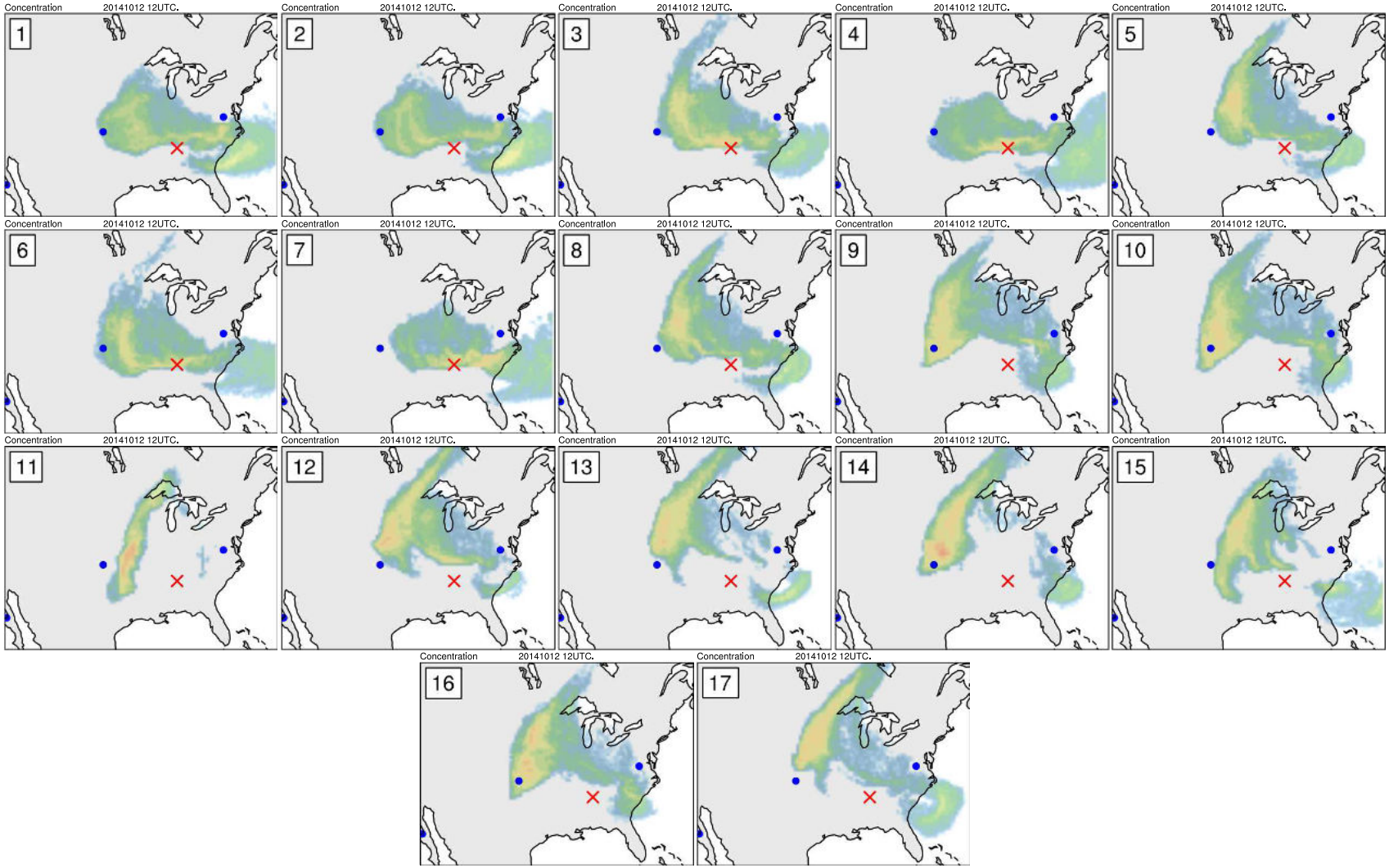
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Plume Ensemble Members

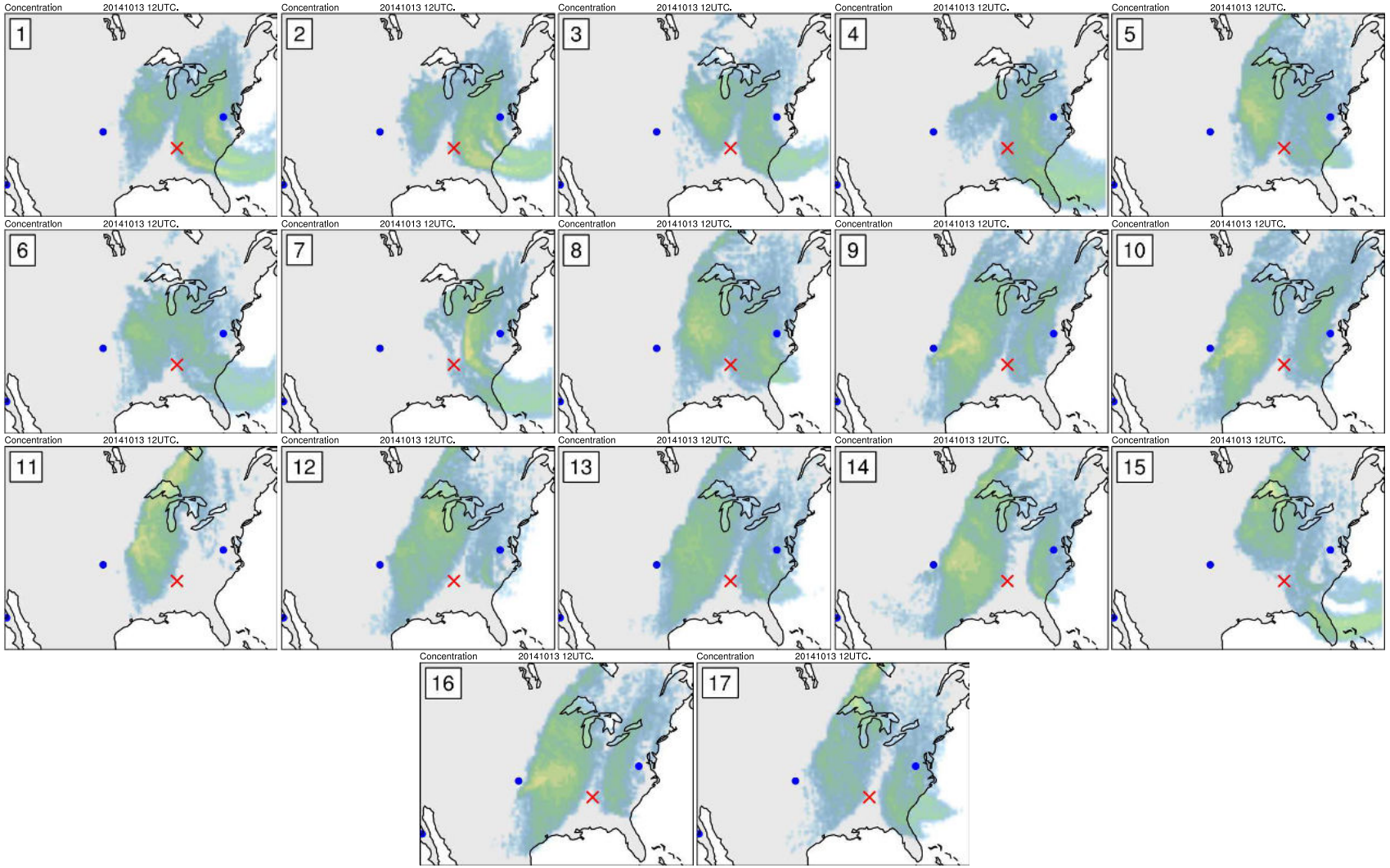
Releases from LOC4: on 12 Oct. 2014



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Plume Ensemble Members

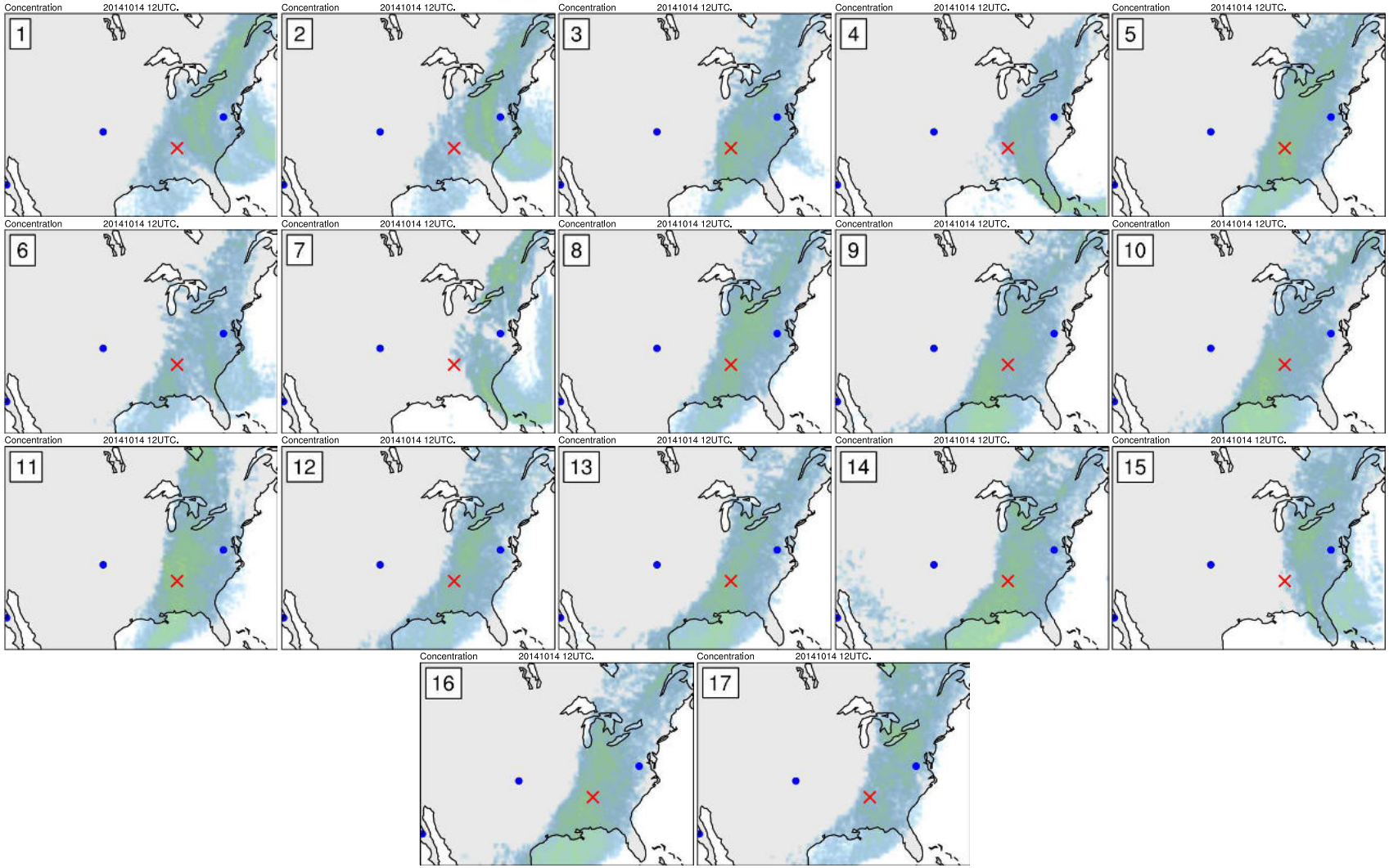
Releases from LOC4: on 13 Oct. 2014



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Plume Ensemble Members

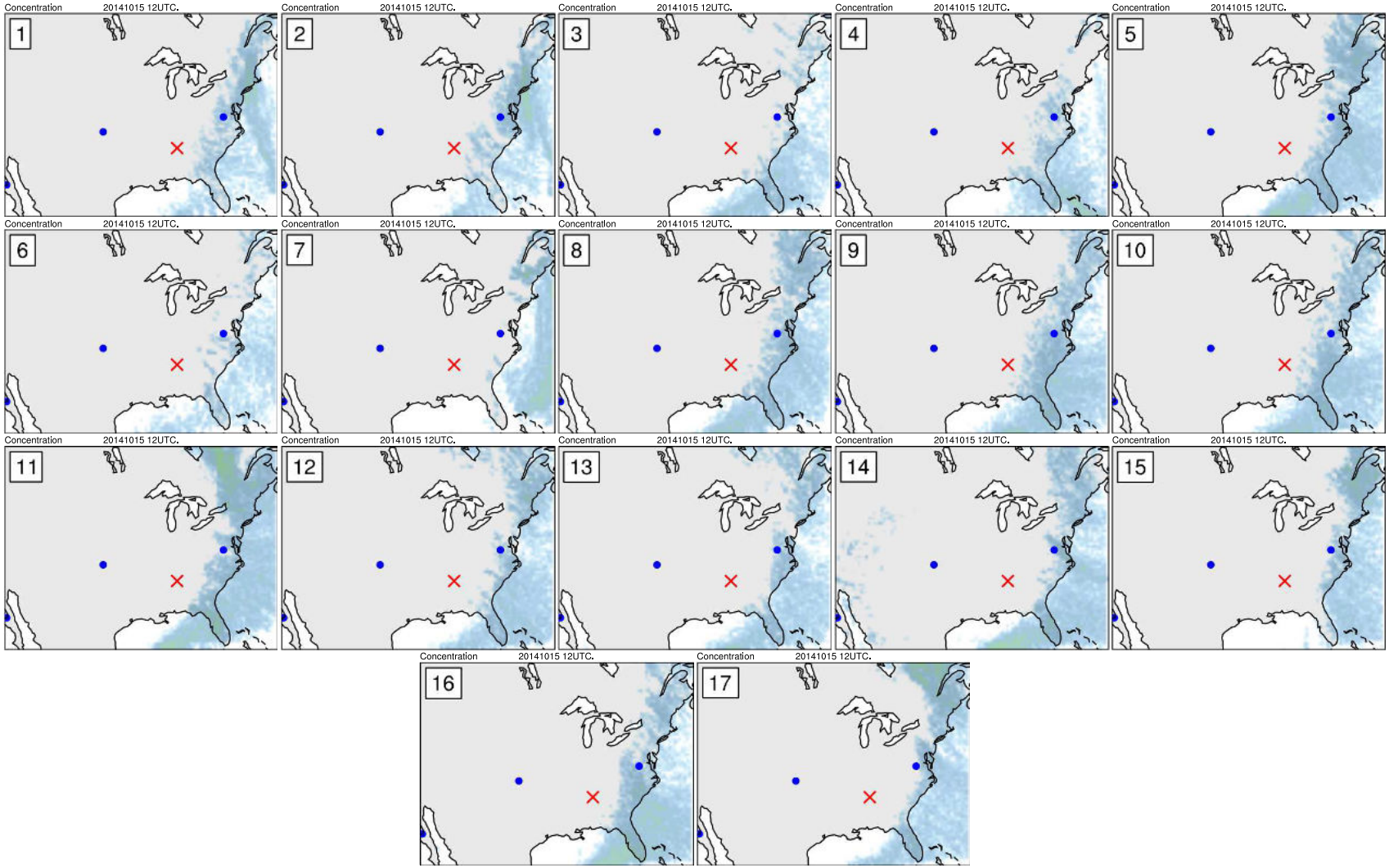
Releases from LOC4: on 14 Oct. 2014



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Plume Ensemble Members

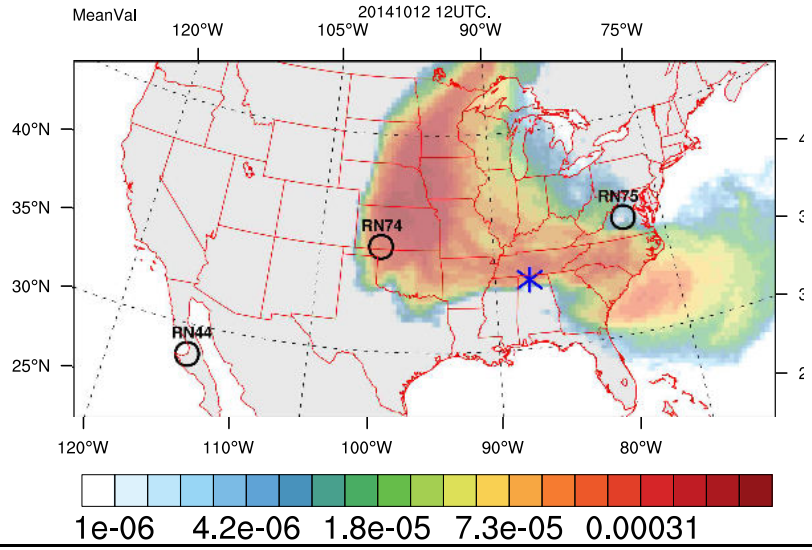
Releases from LOC4: on 15 Oct. 2014



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Forward Plume Statistical Charts

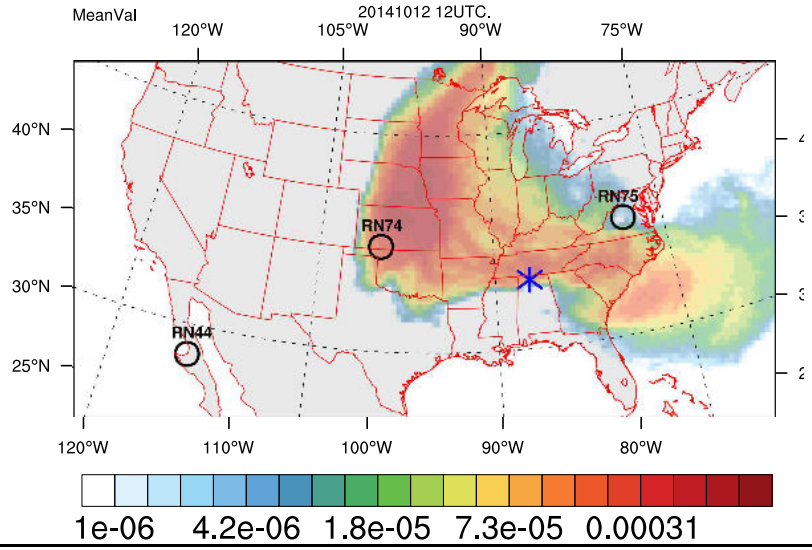
Mean Value



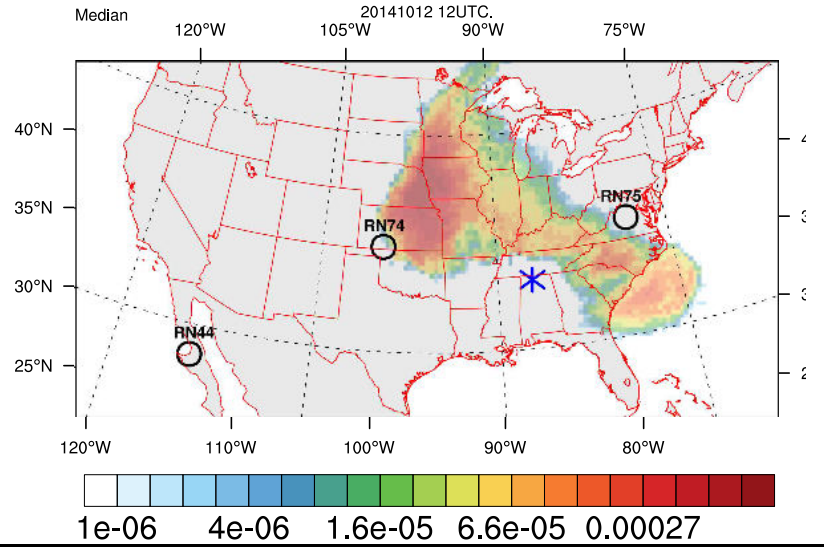
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Forward Plume Statistical Charts

Mean Value



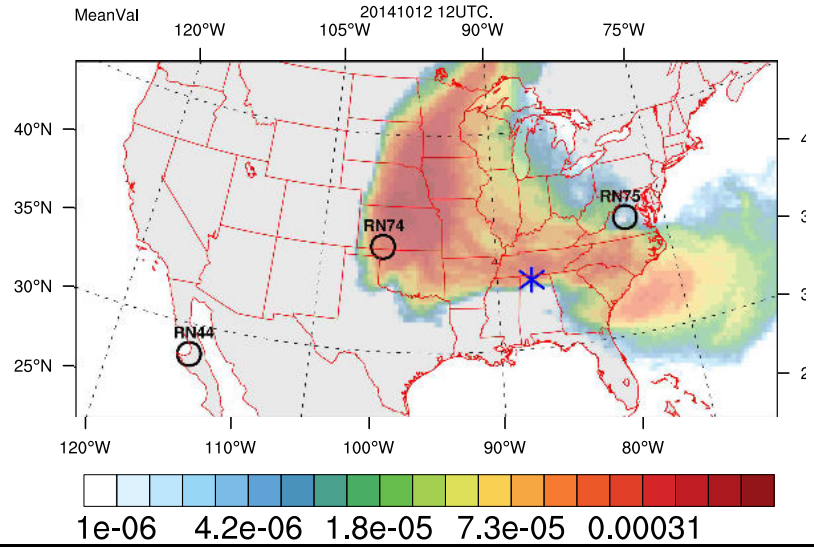
Median Value



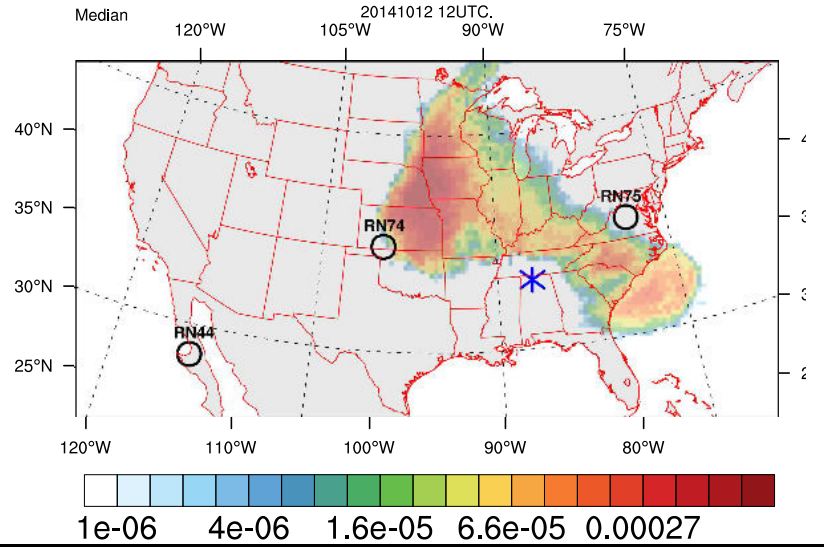
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Forward Plume Statistical Charts

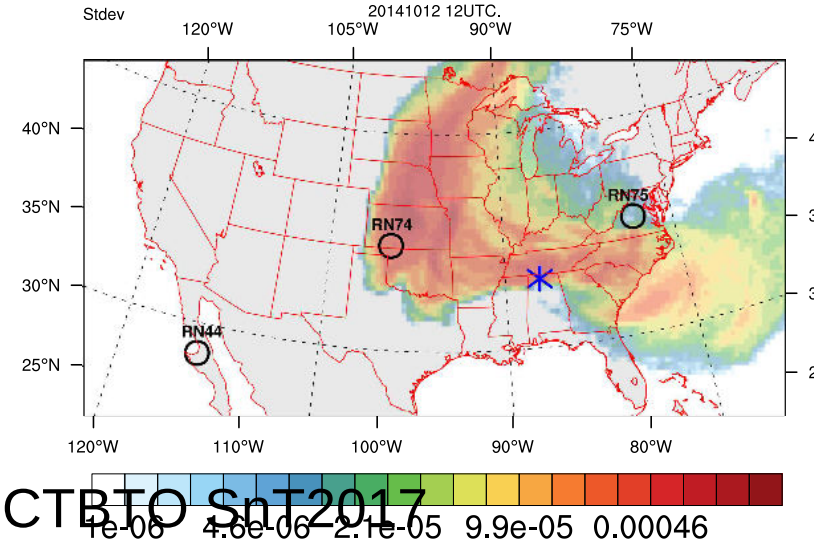
Mean Value



Median Value



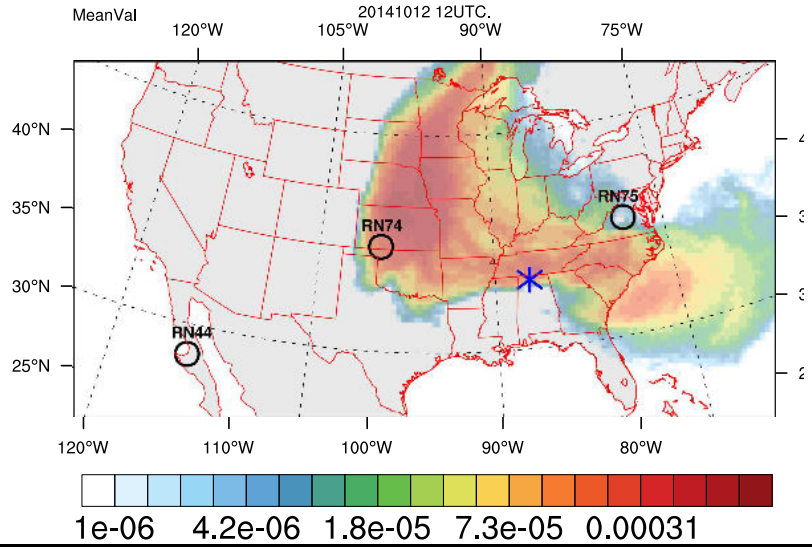
Standard deviation



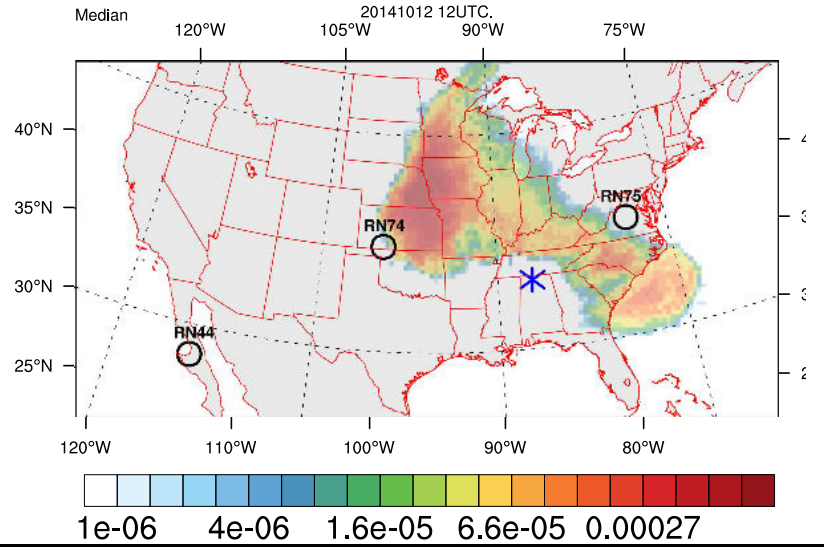
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Forward Plume Statistical Charts

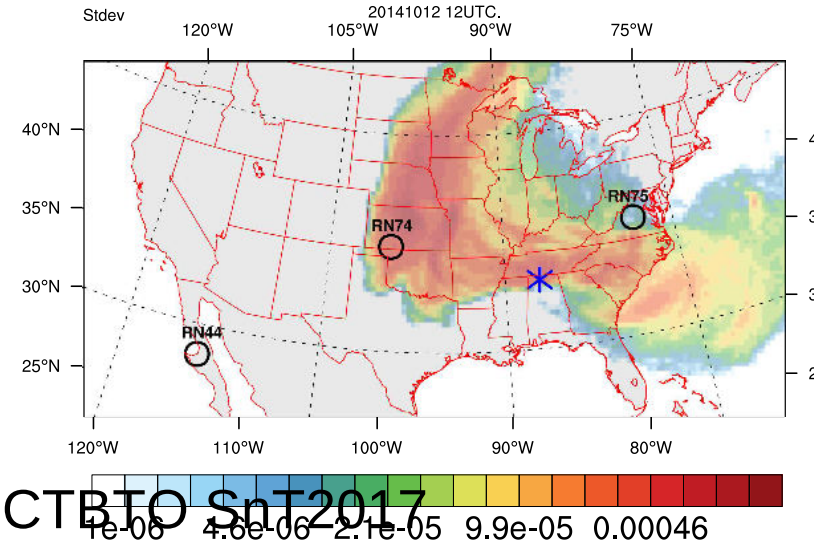
Mean Value



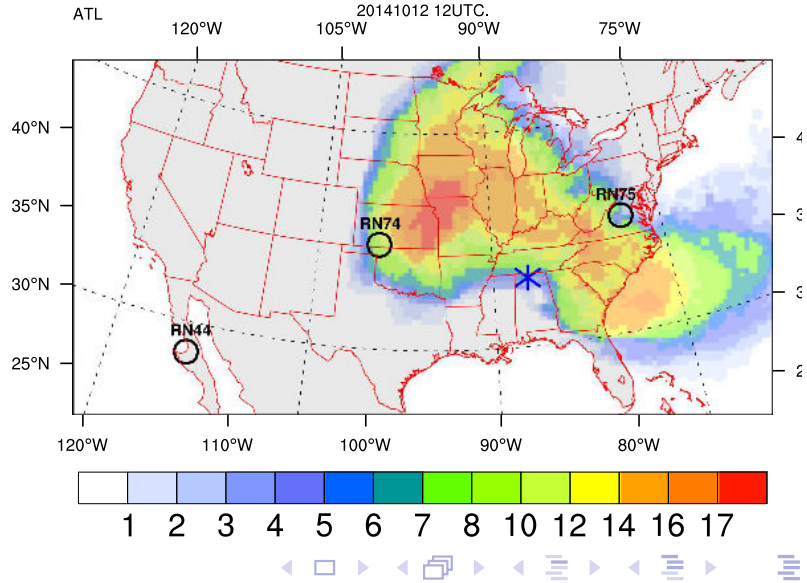
Median Value



Standard deviation

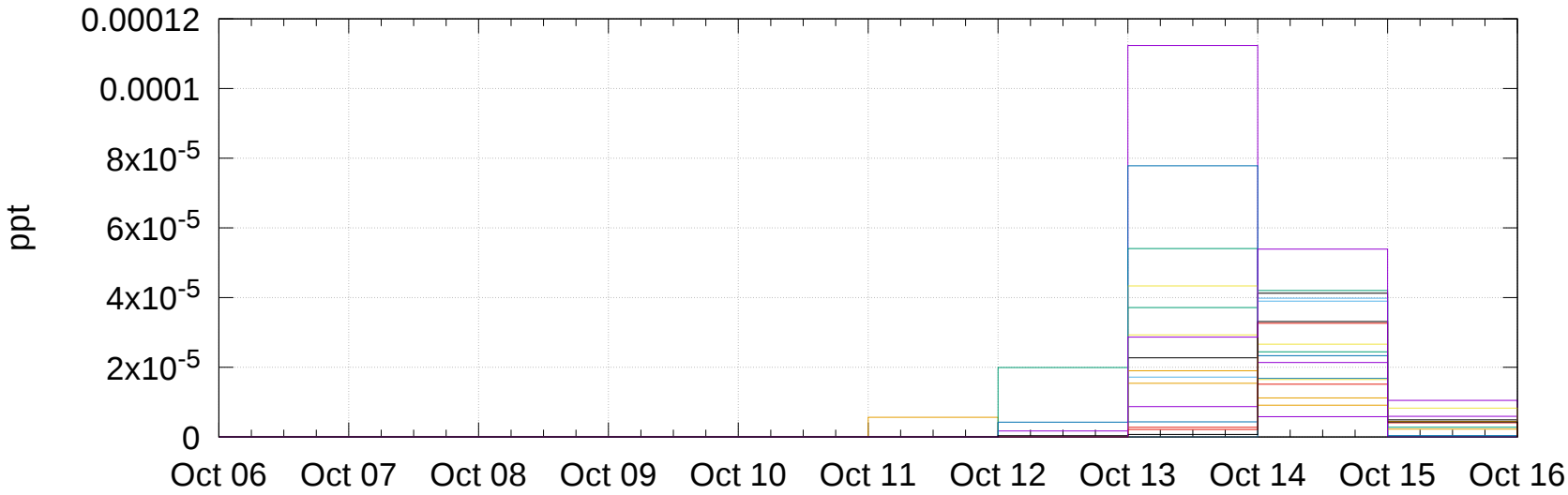


Agreement Threshold level



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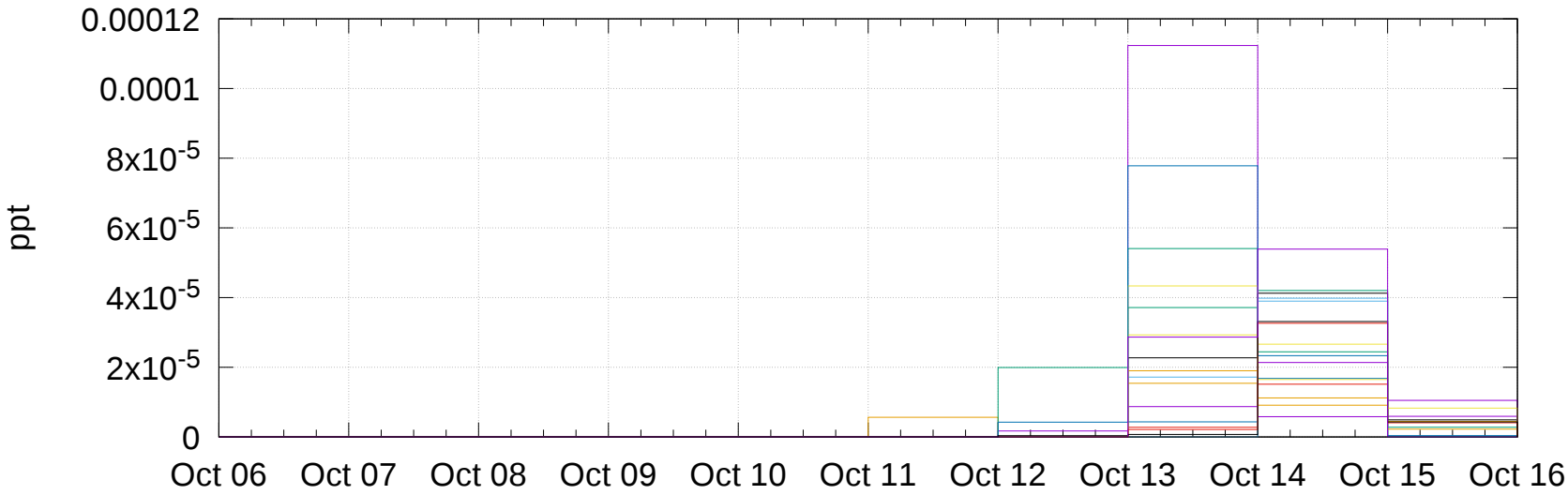
Uncertainties in Synthetic Concentrations



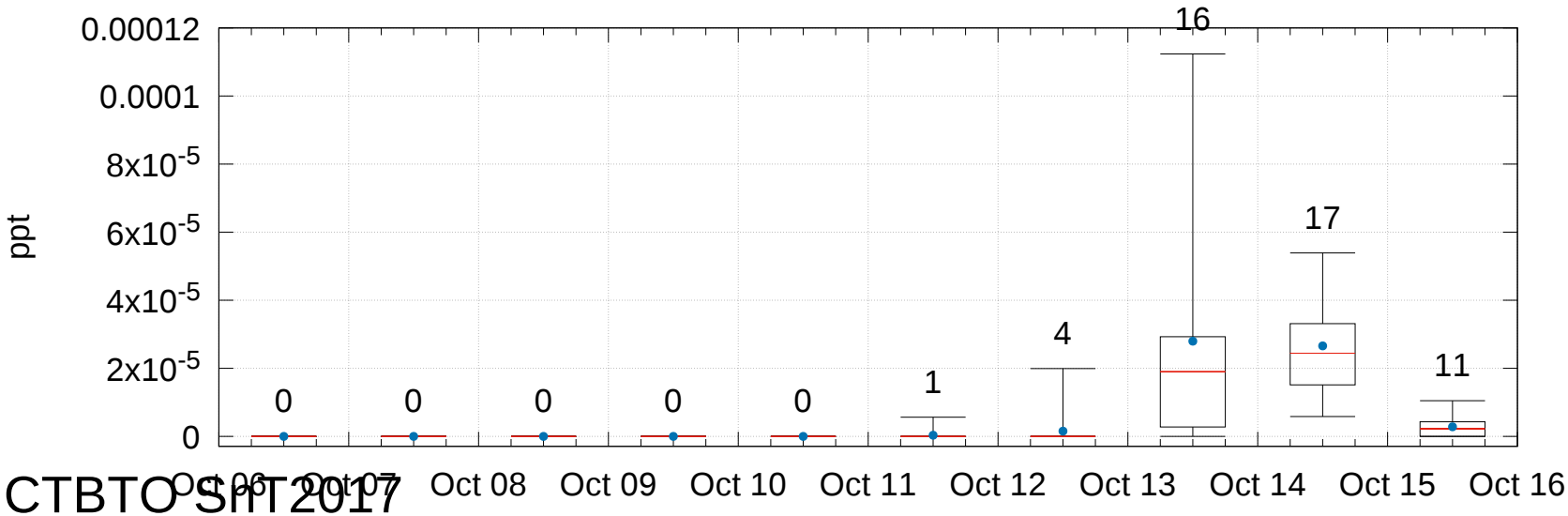
^{133} *Xenon* Concentrations of releases from LOC4 at RN75.

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Uncertainties in Synthetic Concentrations



^{133}*Xenon* Concentrations of releases from LOC4 at RN75.



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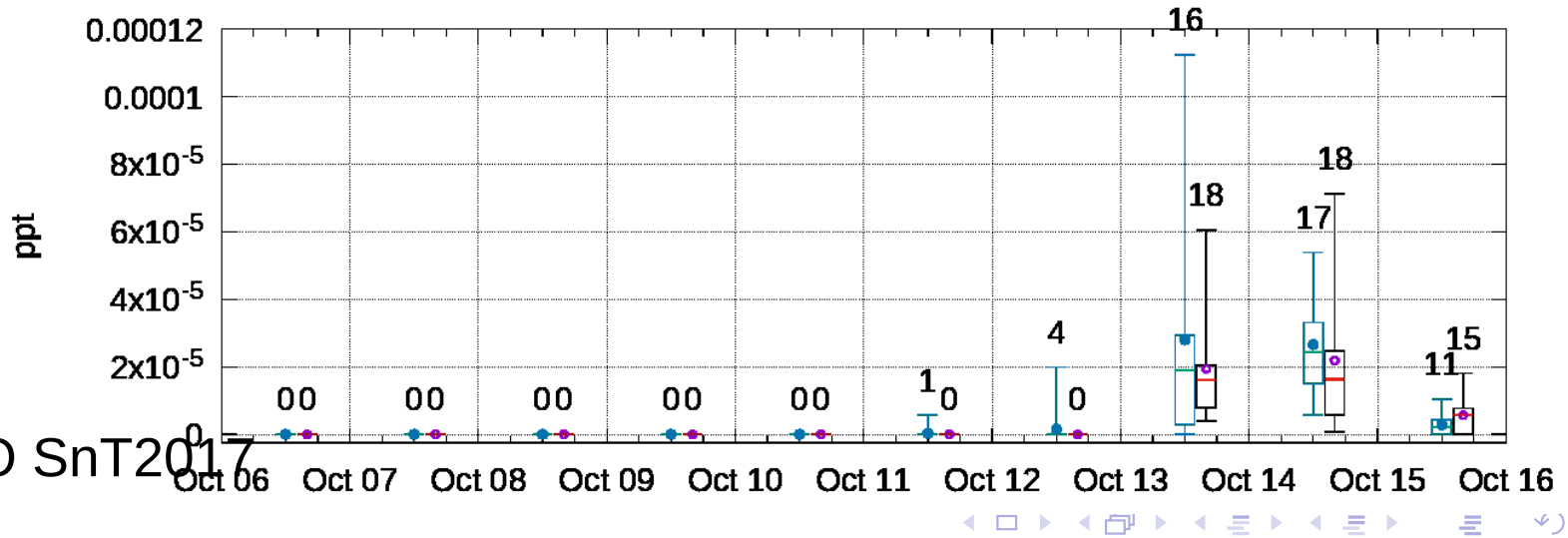
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Bayes' Theorem

$$P(M|D,I) = \frac{P(M|I)P(D|M,I)}{P(D|I)} \quad (1)$$

$P(M|I)$: *prior probability density function*
$P(D|M,I)$: *likehood function*
$P(M|D,I)$: posterior probability density.

$$P(D|M,I) \propto exp(-0.5 \sum_{j=1} \frac{(C_{obs} - C_{est})^2}{\sigma_{obs}^2 + \sigma_{est}^2})$$



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Ensemble Mean PDF

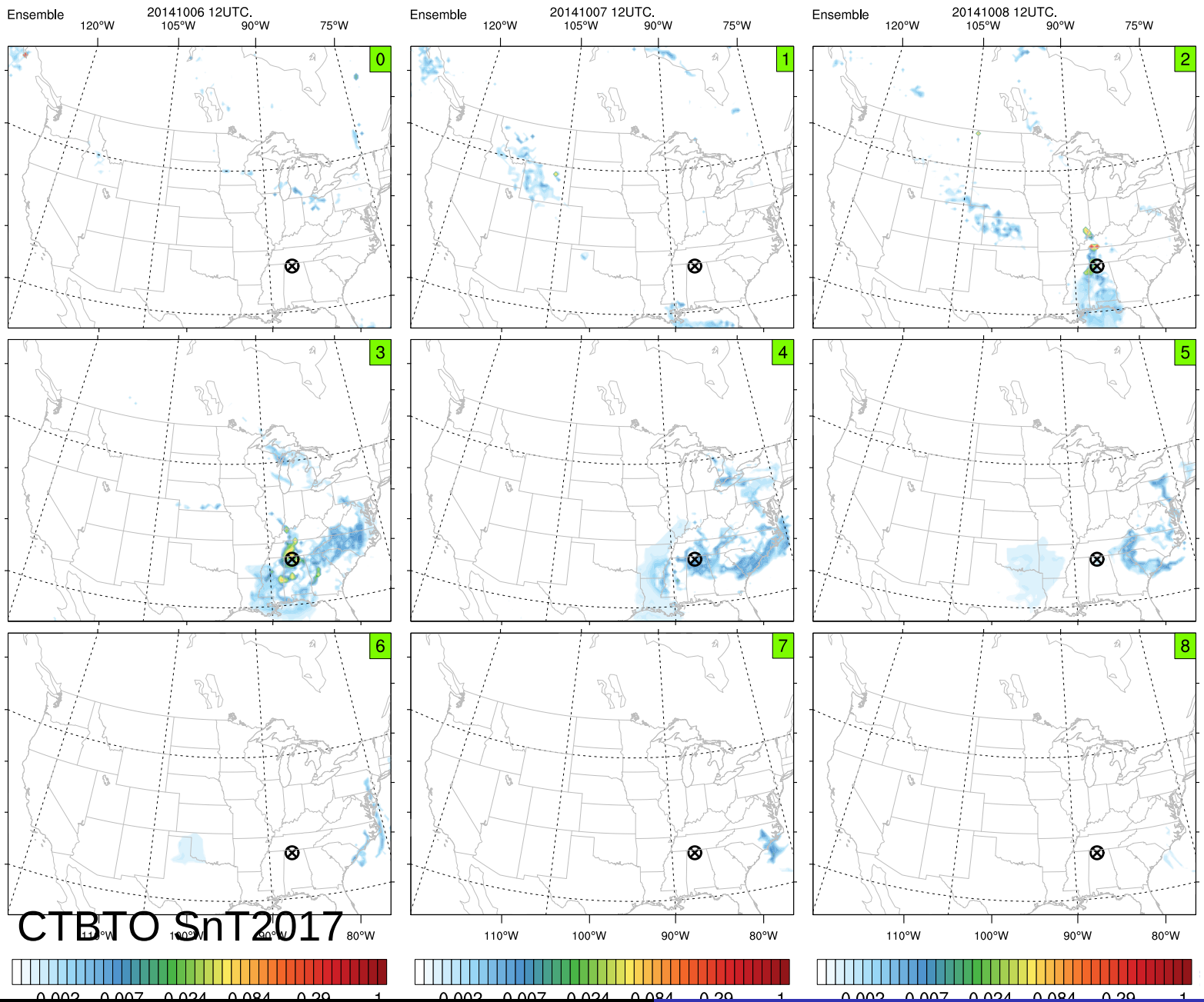
$$P(S) = \sum_{k=1}^{N} P(S|M_k)P(M_k) \tag{2}$$

$P(S|M_k)$: the probability of the Source S given a Model M_k.

$P(M_k)$: the probability of model M_k.

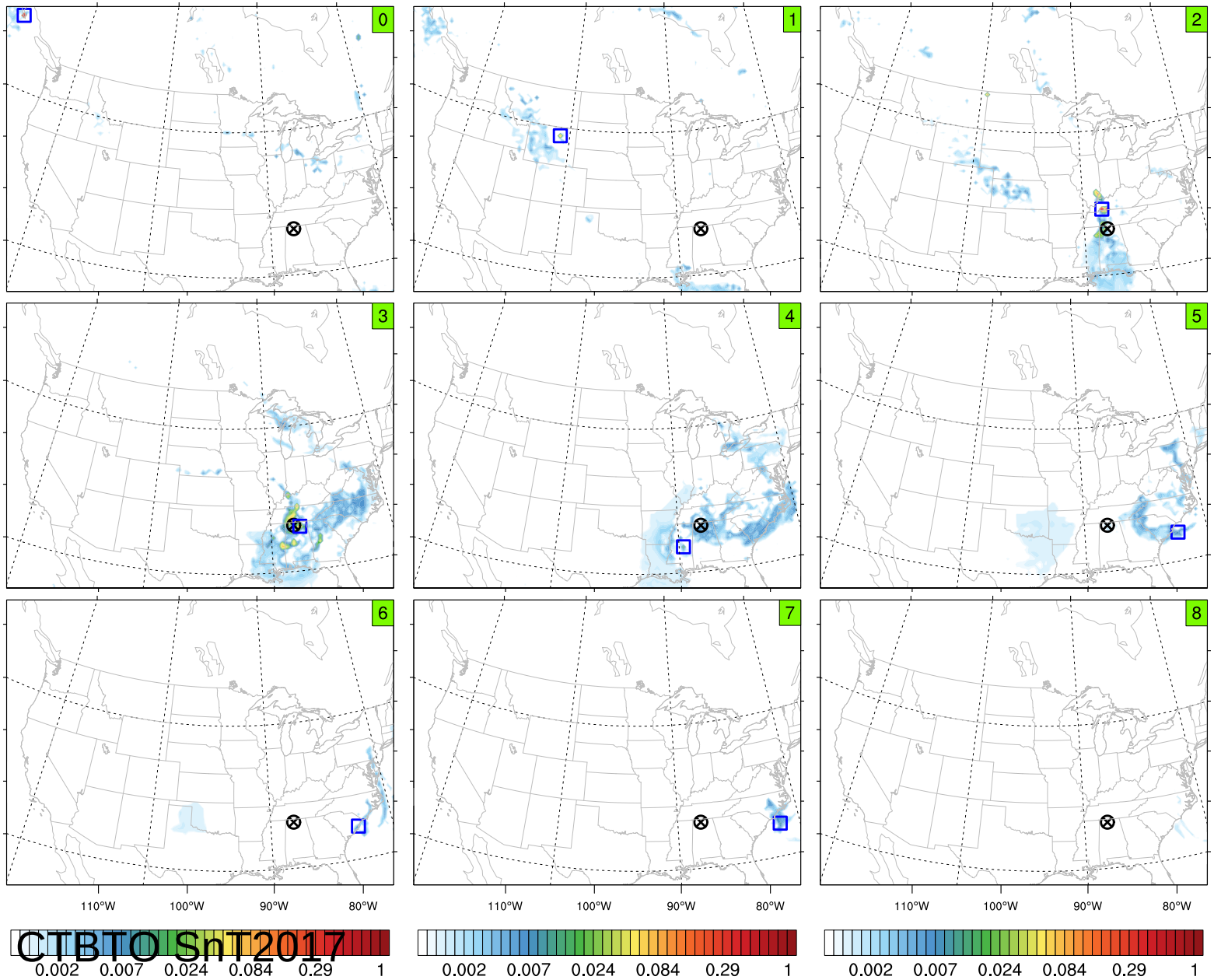
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Time Evolution Ensemble mean of Posterior PDF

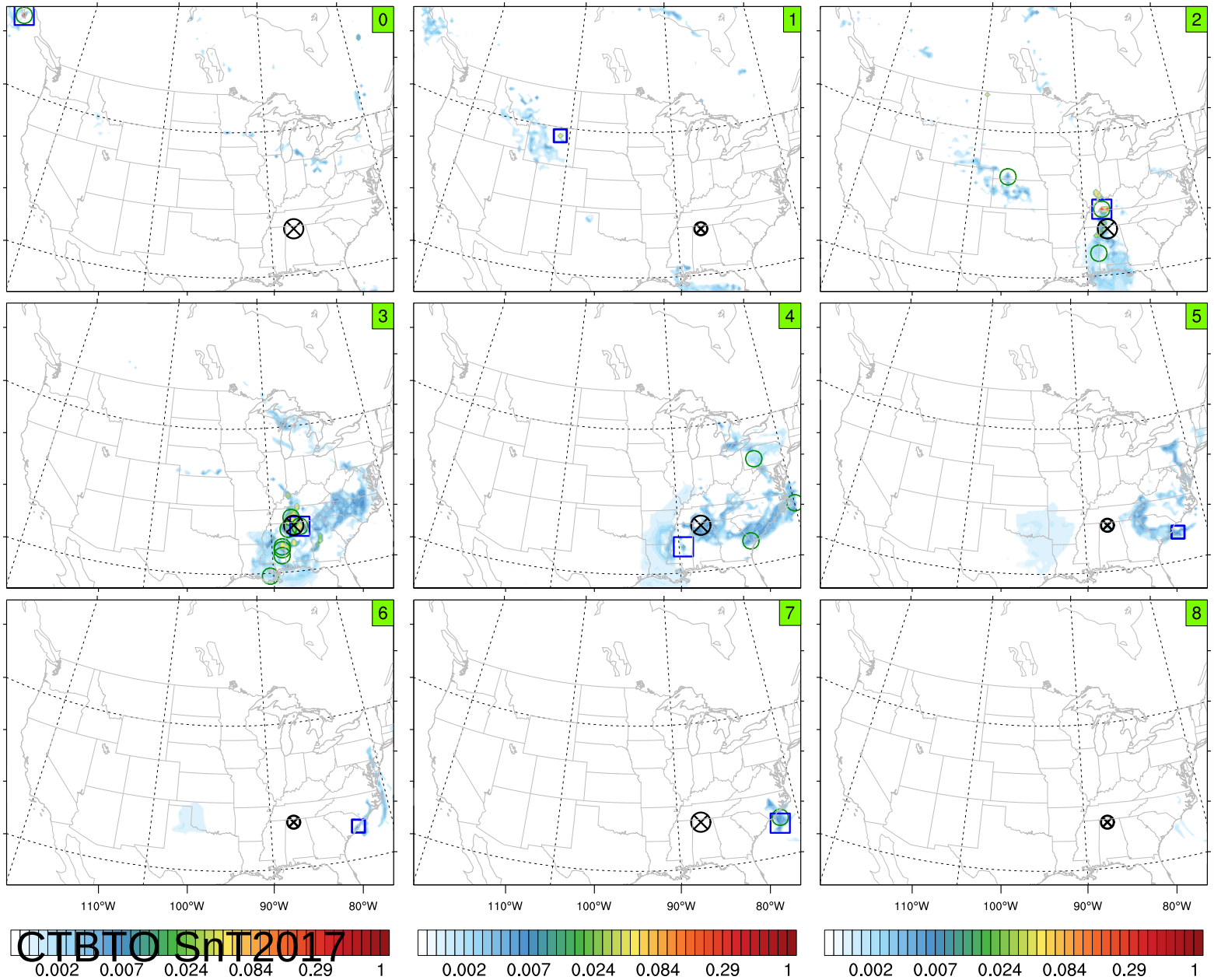


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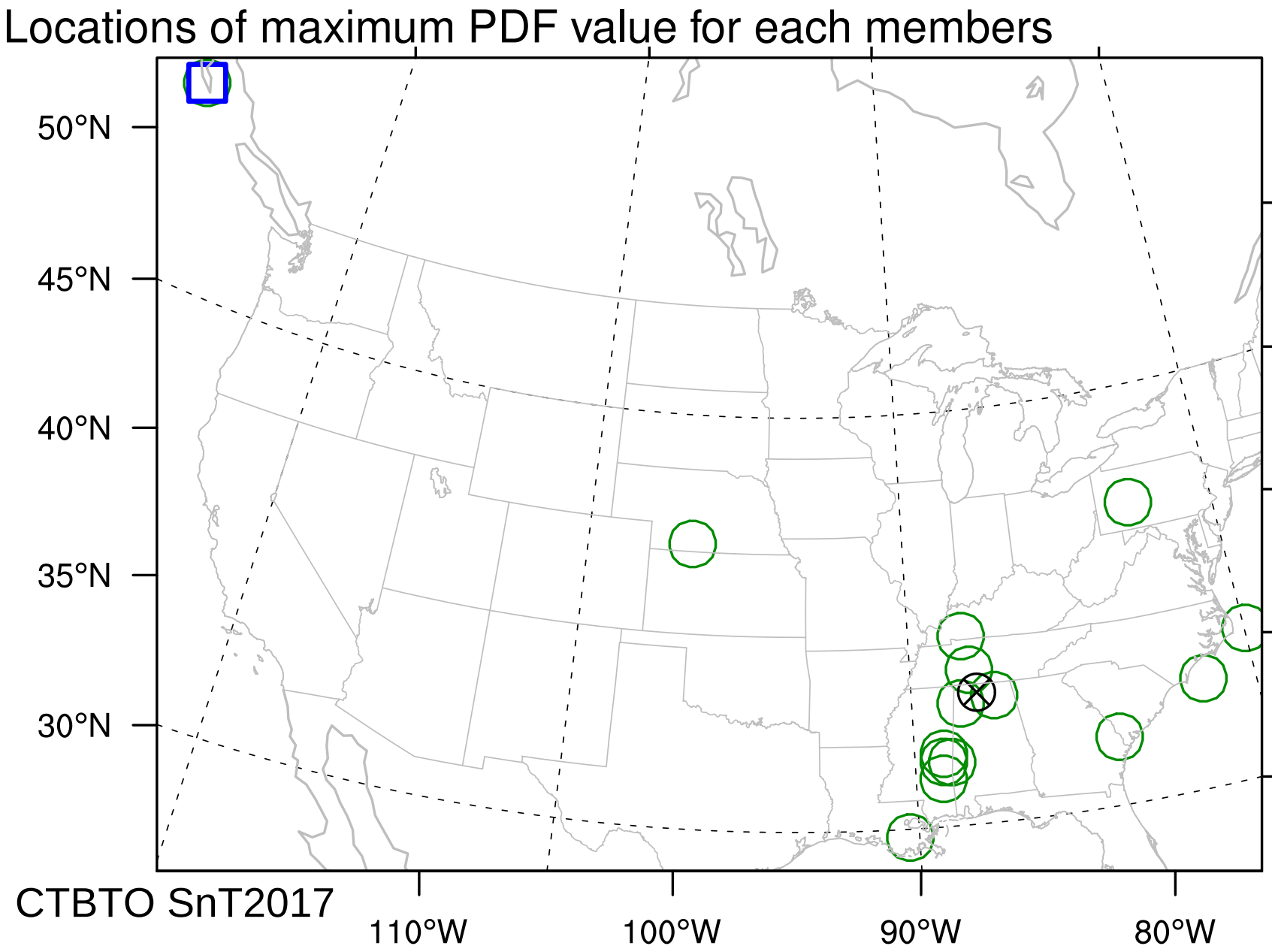
Ensemble mean of Posterior PDF



Ensemble mean of Posterior PDF

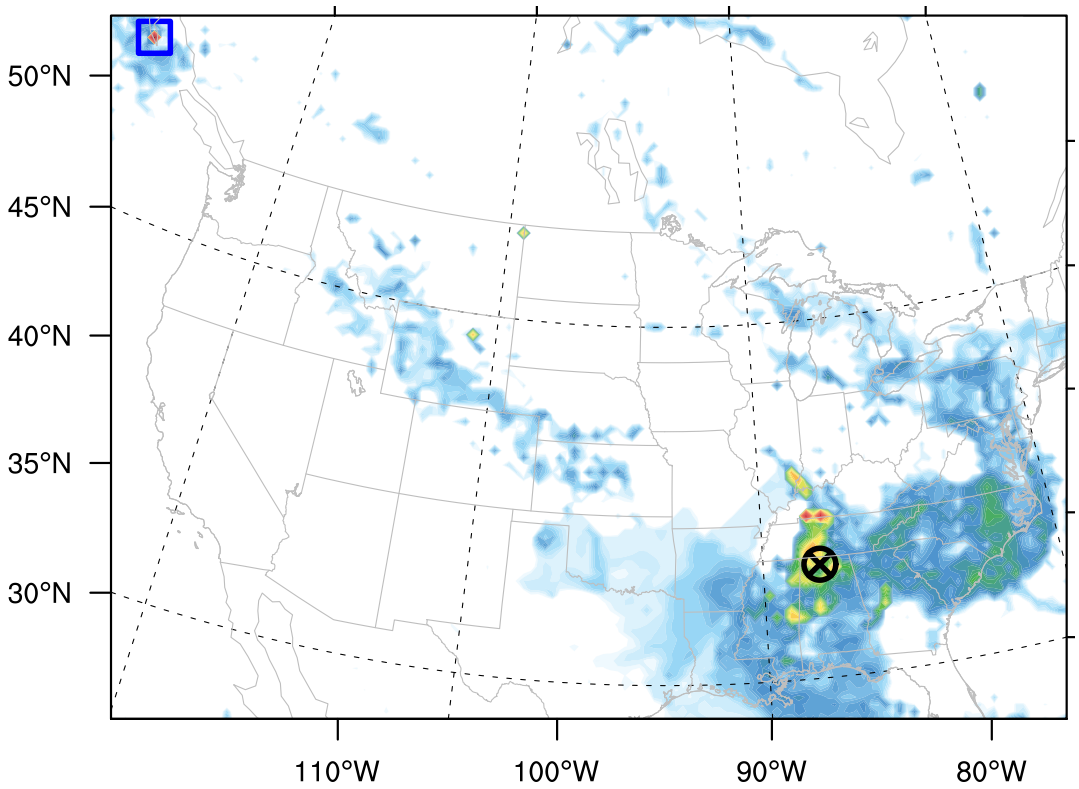


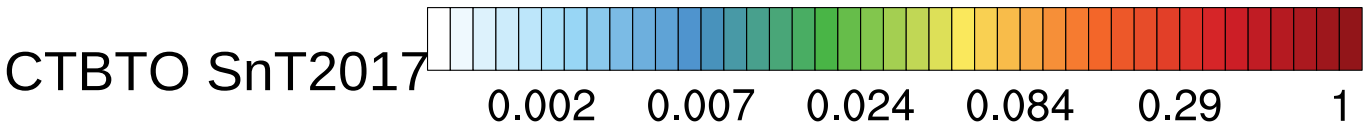
Ensemble of Source Locations



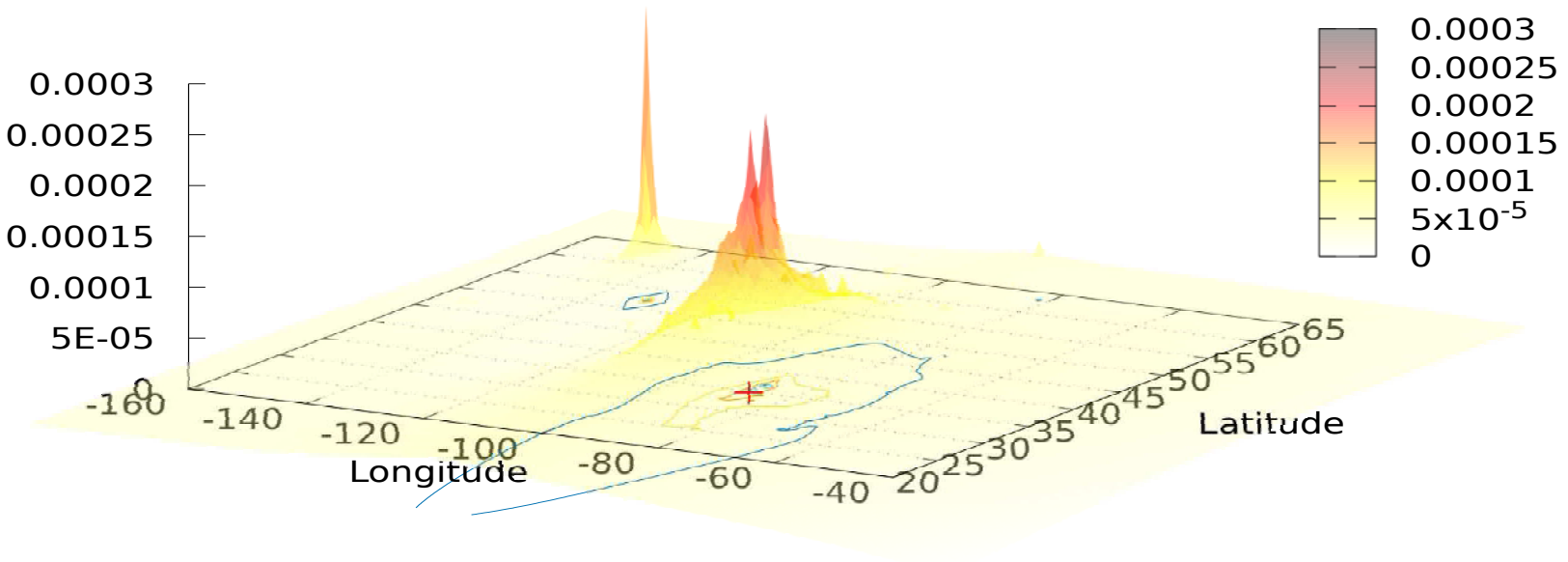
Spatial Marginal of ensemble mean of posterior PD

$$P_m(x_i, y_j) = \sum_{k=1}^{N} P_{i,j,k} \tag{3}$$



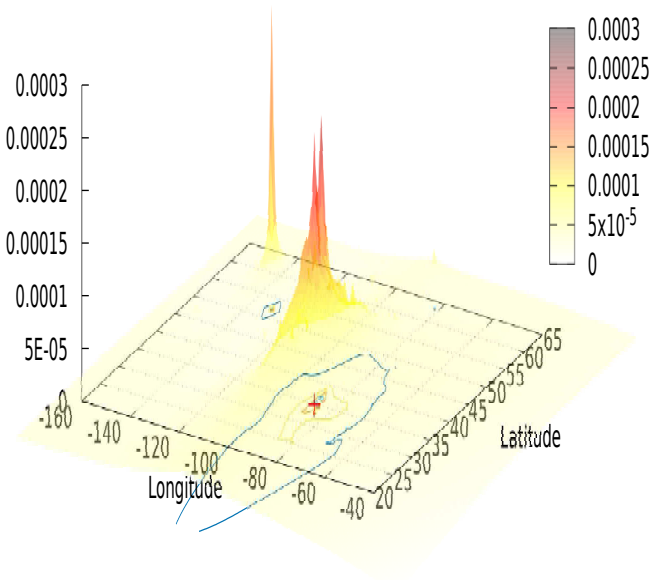


Spatial Marginal of ensemble mean of Posterior PD



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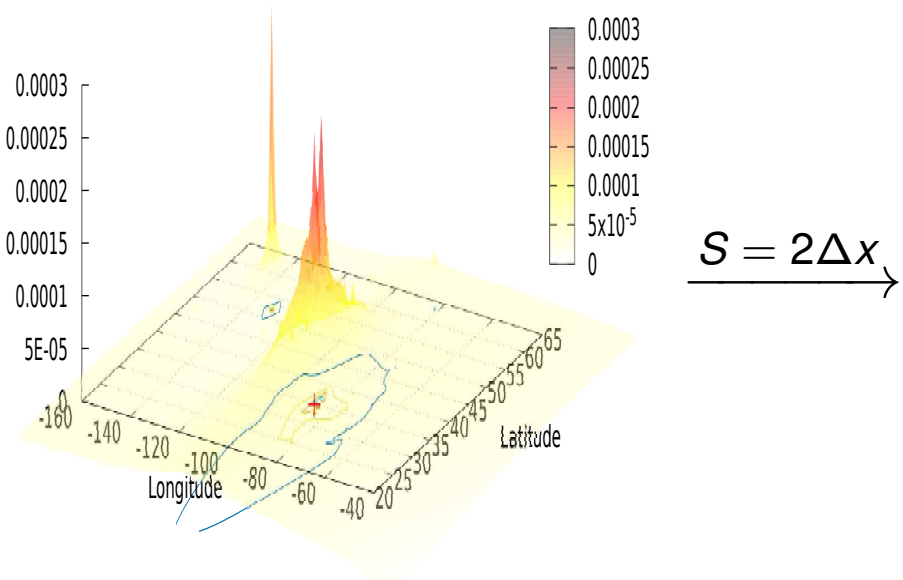
Smoothing by using Kernel Density



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Smoothing by using Kernel Density

$$P_{ms}(x_i, y_j) = \sum_{l=1}^{m} \sum_{q=1}^{n} \frac{P_m(x_i, y_j)}{2\pi S^2} \times exp\left(-0.5 \frac{(x_i - x_l)^2 + (y_j - y_q)^2}{S^2}\right) \tag{4}$$

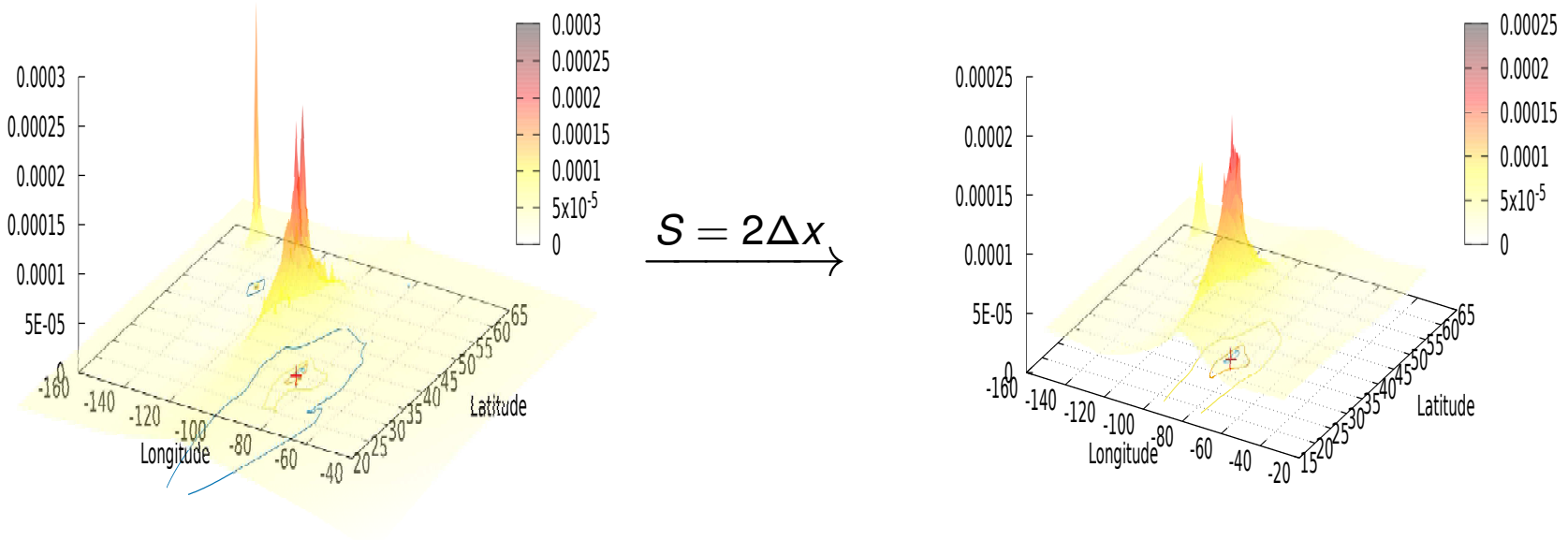


$S = 2\Delta x$

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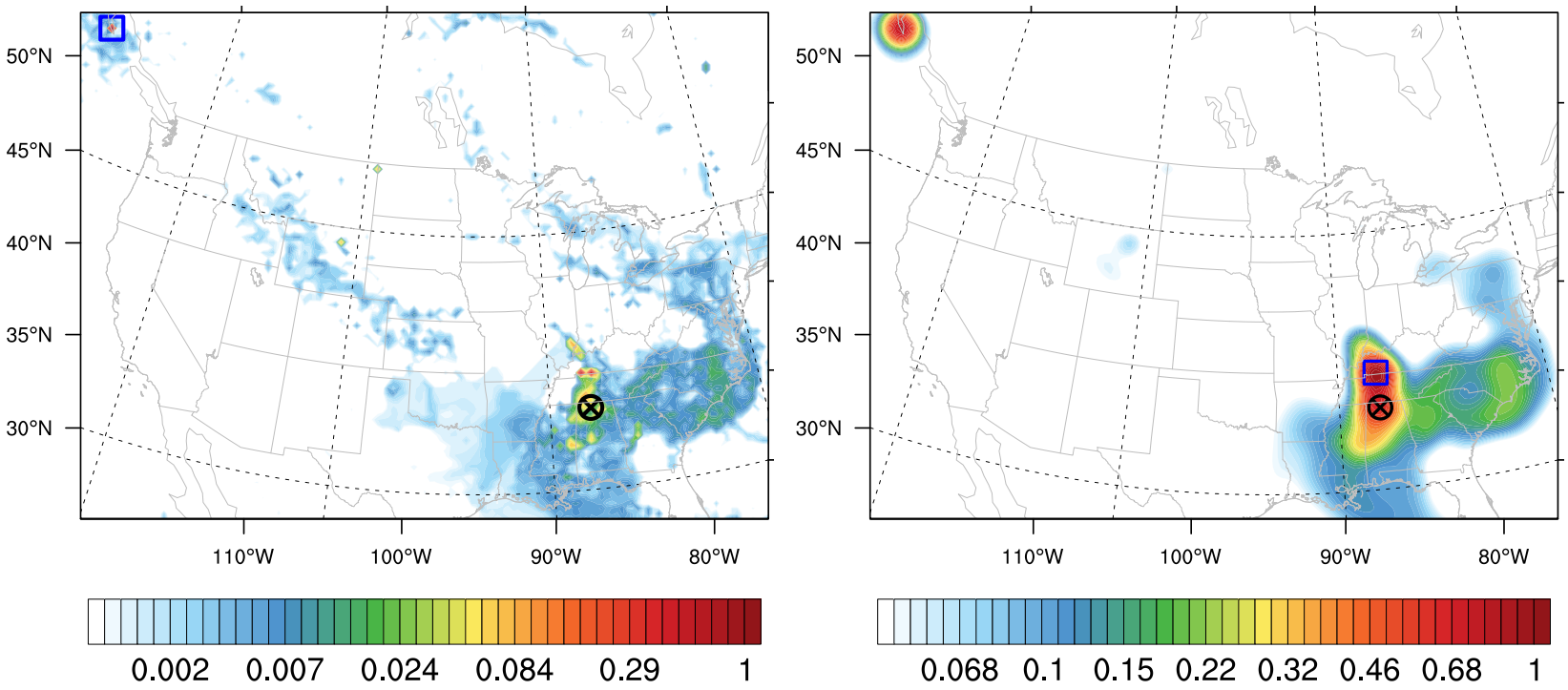
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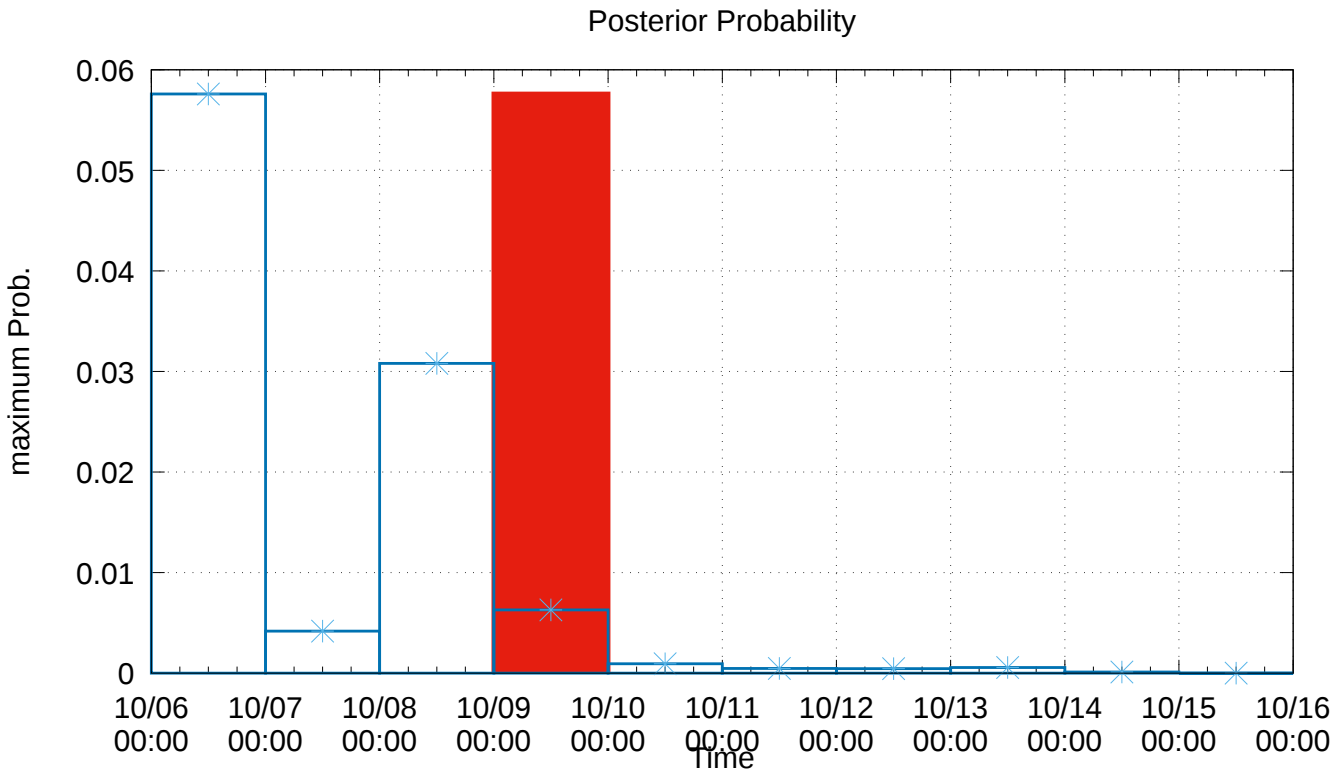
Smoothing by using Kernel Density



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What about time of Release?

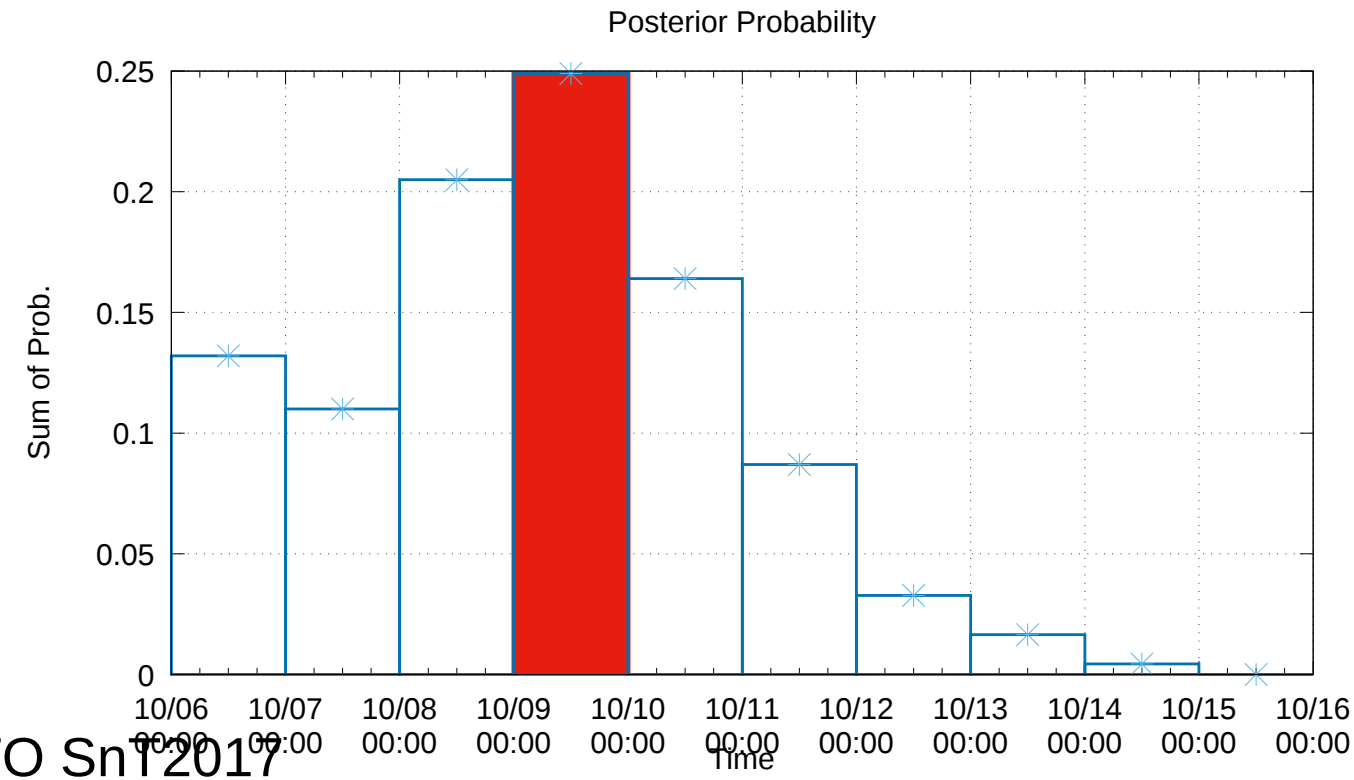
Maximum value of ensemble mean of Posterior PDF



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Temporal Marginal of ensemble mean of Posterior PDF

$$P_m(t_k) = \sum_{i=1}^{m} \sum_{j=1}^{n} P_{i,j,k} \tag{5}$$

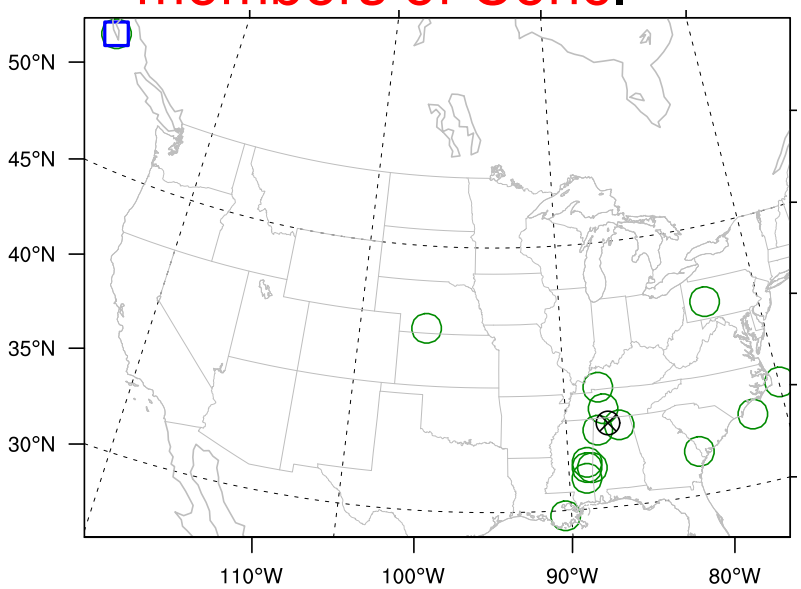


CTBTO Sn12017

The variance of ensemble member solutions

How much is this variance related to the uncertainties in concentrations or meteorological fields?

Method1:
members of SRS
+
members of Conc.

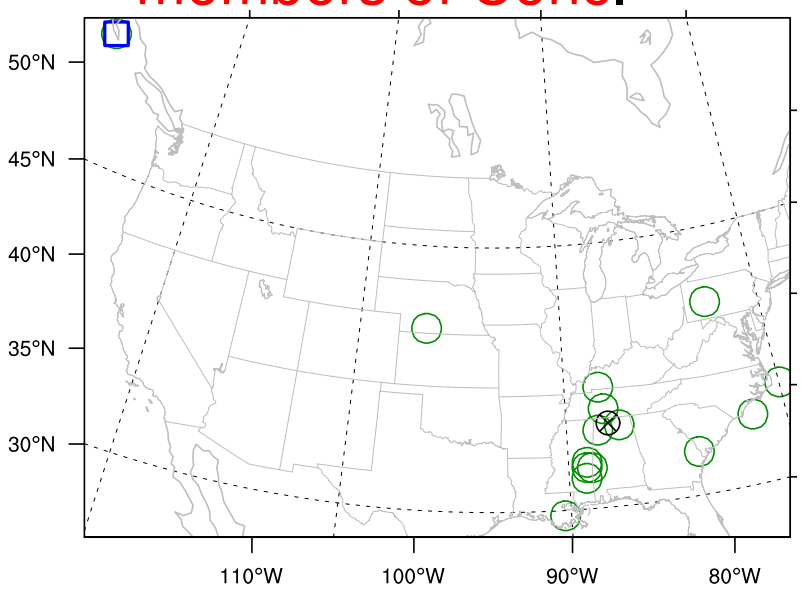


CTBTO SnT2017

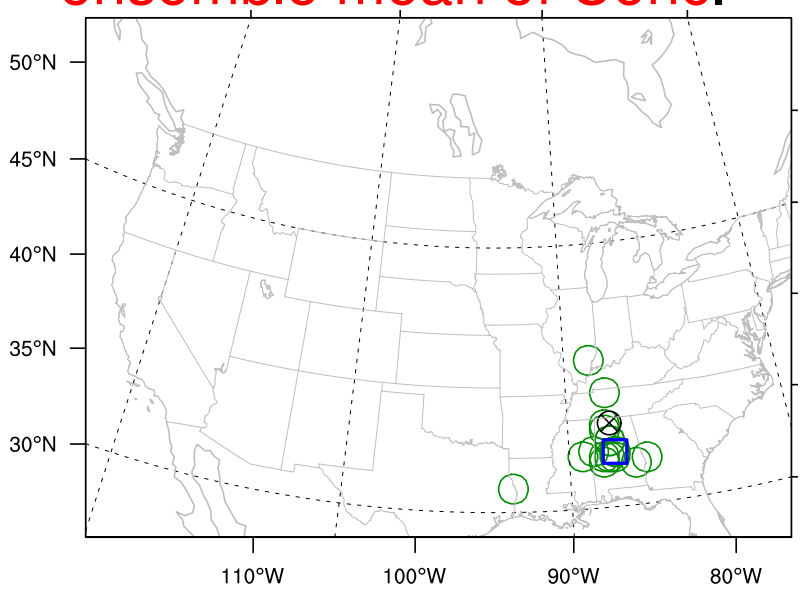
The variance of ensemble member solutions

How much is this variance related to the uncertainties in concentrations or meteorological fields?

Method1:
members of SRS
+
members of Conc.



Method2:
members of SRS
+
ensemble mean of Conc.

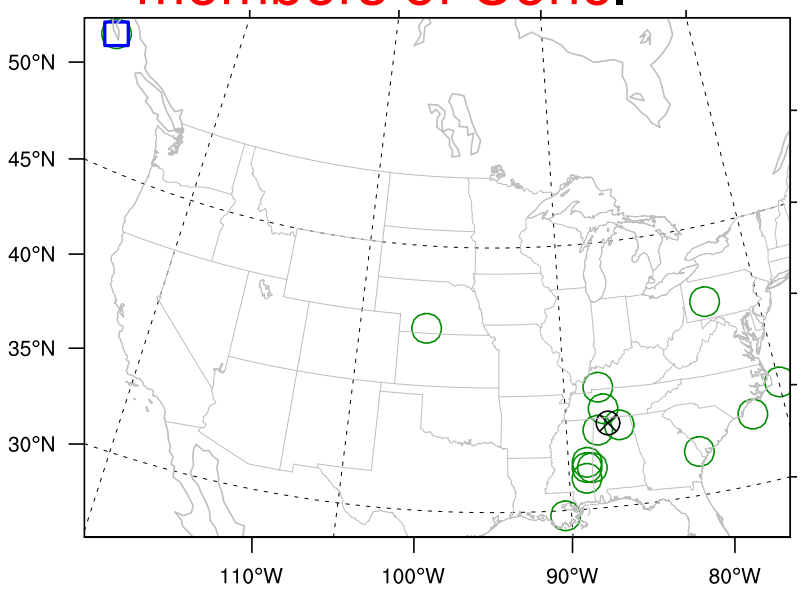


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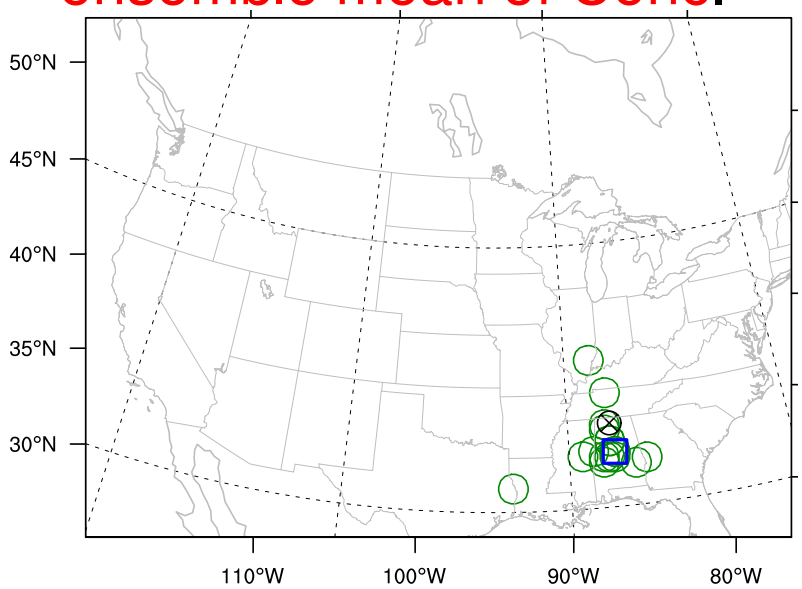
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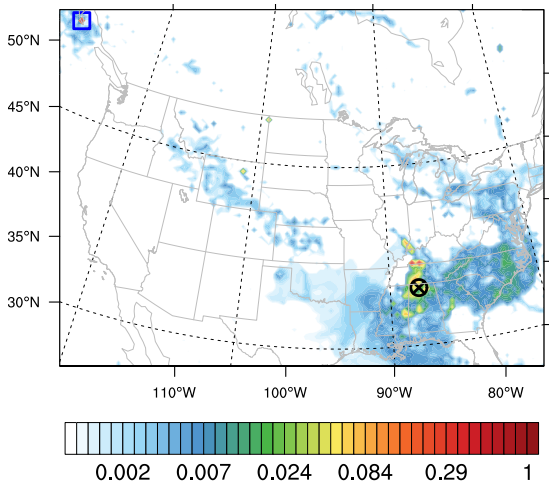
Method2:
members of SRS
+
ensemble mean of Conc.



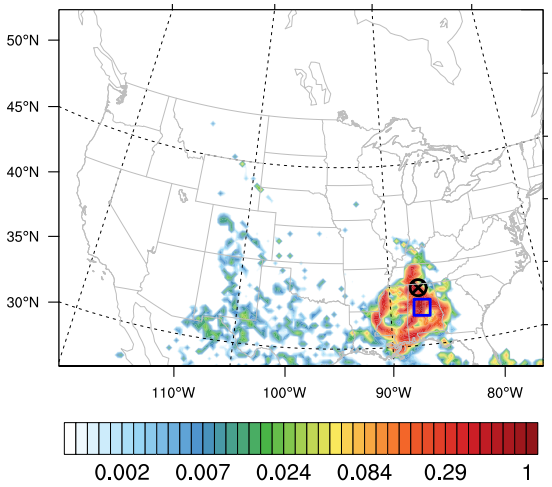
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Three Methods for Source Parameter Estimation

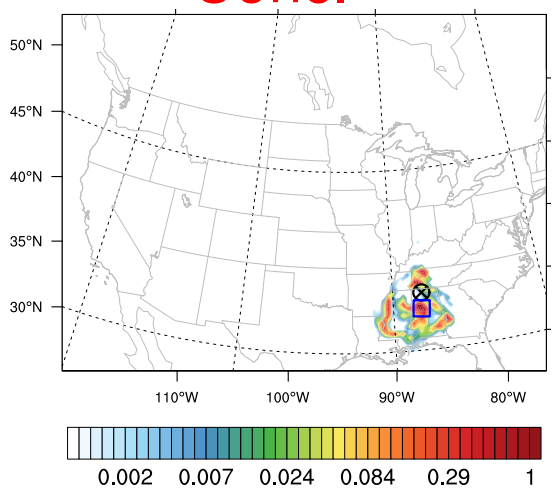
Method1:
members of SRS
+
members of Conc.



Method2:
members of SRS
+
ensemble mean of Conc.

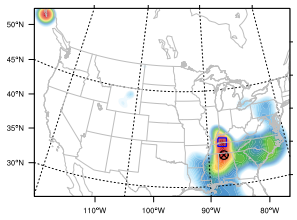
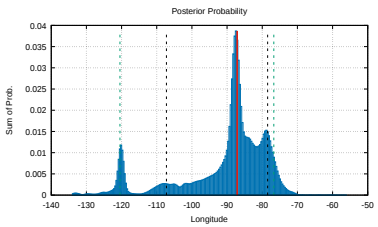
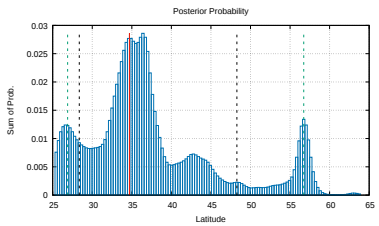
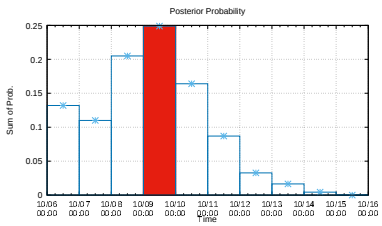
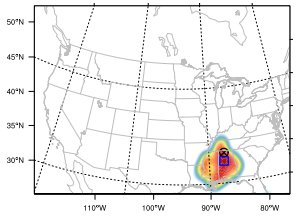
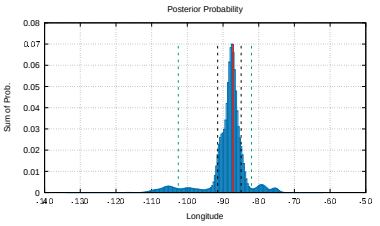
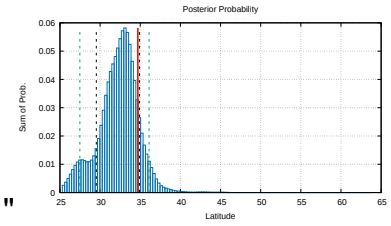
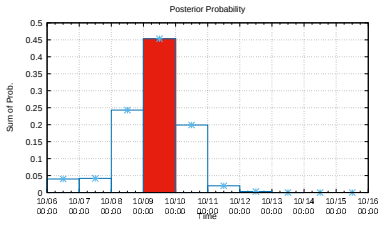
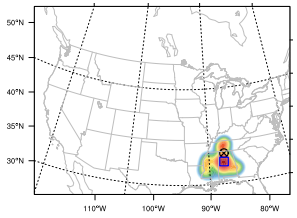
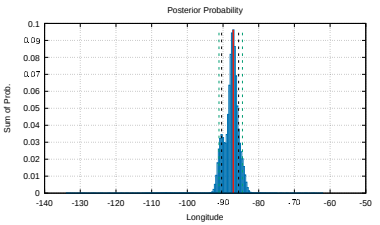
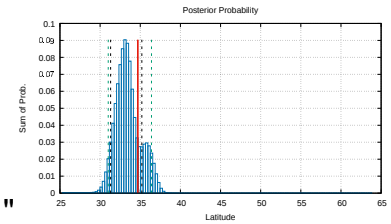
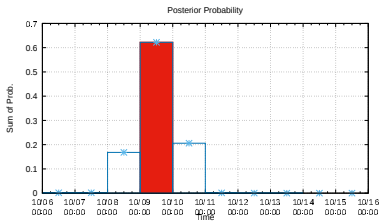


Method3:
ensemble mean of SRS
+
ensemble mean of Conc.



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Three Methods for Source Parameter Estimation

	Spatial	Longitudinal	Latitudinal	Temporal
Method 1				
	Error	δX=0.3dx	$\delta Y = -6.1dy$	$\delta T = 0$ step
	credible interval 75%	$\Delta_{75} X = 44.6dx$	$\Delta_{75} Y = 29.9dy$	$\Delta_{75} T = \pm 2.5dt$
	credible interval 90%	$\Delta_{90} X = 67.7dx$	$\Delta_{90} Y = 44.8dy$	$\Delta_{90} T = \pm 3.5dt$
Method 2	Spatial	Longitudinal	Latitudinal	Temporal
				
	Error	$\delta X = 0.3dx$	$\delta Y = 3.9dy$	$\delta T = 0$ step
	credible interval 75%	$\Delta_{75} X = 9.6dx$	$\Delta_{75} Y = 8.0dy$	$\Delta_{75} T = \pm 1.5dt$
	credible interval 90%	$\Delta_{90} X = 30.2dx$	$\Delta_{90} Y = 12.9dy$	$\Delta_{90} T = \pm 2.5dt$
Method 3	Spatial	Longitudinal	Latitudinal	Temporal
				
	Error	$\delta X = 0.3dx$	$\delta Y = 3.9dy$	$\delta T = 0$ step
	credible interval 75%	$\Delta_{75} X = 7.0dx$	$\Delta_{75} Y = 5.8dy$	$\Delta_{75} T = \pm 1.5dt$
	credible interval 90%	$\Delta_{90} X = 9.6dx$	$\Delta_{90} Y = 8.0dy$	$\Delta_{90} T = \pm 1.5dt$

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Error in Source Parameter Determination

LOCATION	LONG (dx)	LAT (dy)	Time (dt)
LOC1	2.3	.5	-1.00
LOC2	-1.9	-2.7	1.00
LOC3	.4	-6.3	1.00
LOC4	.4	4.8	0
LOC5	3.9	6.8	1.00
LOC6	-1.8	21.4	2.00

Table: Error in Estimation

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Uncertainties in Possible Source

LOCATION	LONG (dx)		LAT (dy)		Time (dt)	
	$\Delta_{75}X$	$\Delta_{90}X$	$\Delta_{75}Y$	$\Delta_{90}Y$	$\Delta_{75}T$	$\Delta_{90}T$
LOC1	7.0	15.3	3.9	6.5	1.5	2.5
LOC2	12.0	14.2	6.1	11.4	1.0	2.0
LOC3	7.3	11.3	14.3	17.9	1.5	2.5
LOC4	7.5	9.6	5.3	7.6	1.5	2.0
LOC5	8.6	11.4	11.7	15.8	1.5	2.0
LOC6	12.0	15.2	15.0	22.4	2.0	3.00

Table: Credible Intervals 75% and 90% of posterior PDF

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Conclusions

- For middle latitude region, the atmospheric uncertainties propagate from west to east.
- For Short period simulation, there is a growth of uncertainties with time.
- The atmospheric uncertainties are associated mainly with regions of with baroclinic systems (low pressure and trough regions).
- Ensemble technique can reduces the uncertainty in source Determination,
- Combining the Ensemble Technique and Inverse Method by Bayesian Approach provides us with a method to source uncertainty quantification.

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Thank You

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