Study of Uncertainty Quantification through Machine Learning Techniques

Polynomial Chaos with Neural Networks

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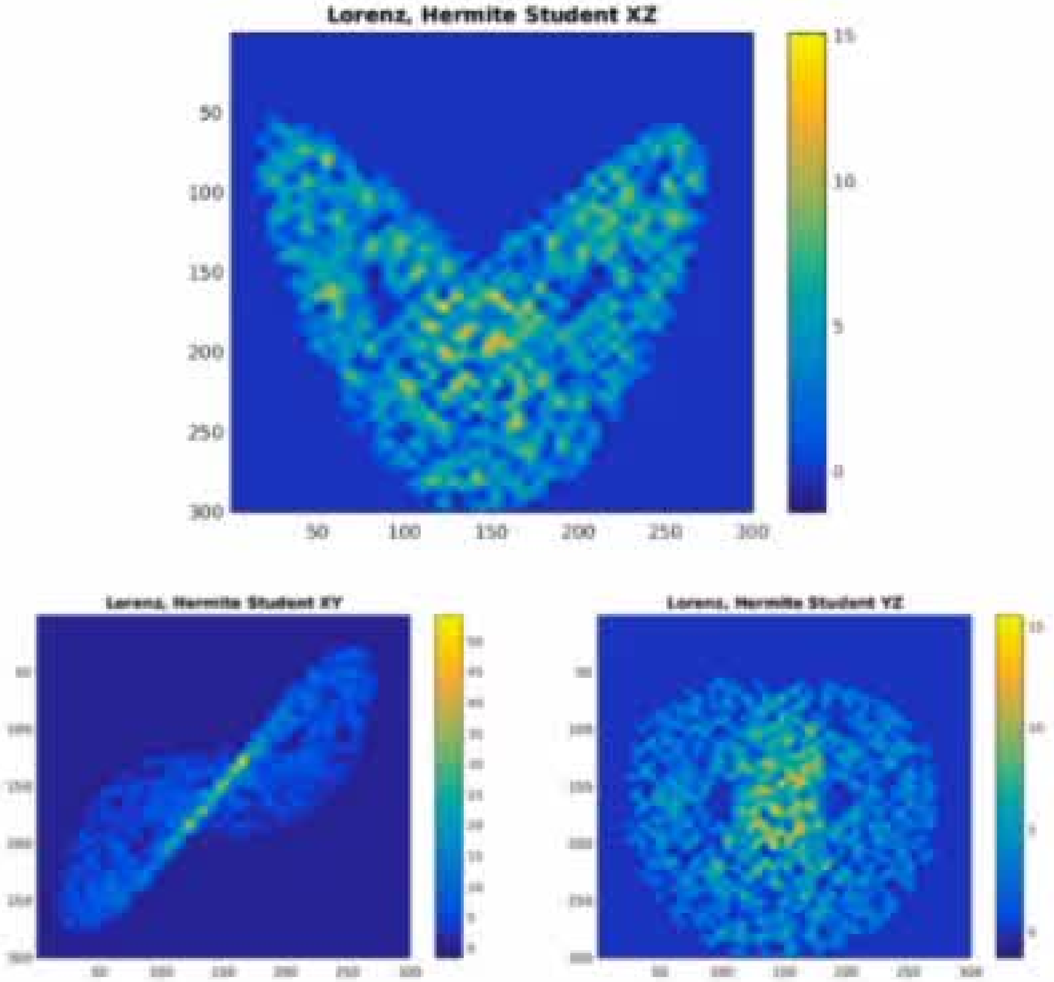
Compute the Future!

VIRGINIA TECH.

The student learns the behaviors of the larger ReLU model in the smaller framework.

- Teacher student training
- Qualitatively closest result



Estimated polynomial for Lorenz System

$$
\begin{aligned}
f(x_1, x_2, x_3) = \max\{0, (&H_1(-0.65382x_1 + 0.0619x_2 - 0.0387x_3) + \\
&H_2(-0.6692x_1 + 0.8177x_2 - 0.5841x_3 - 0.0123) + \\
&H_3(0.4283x_1 + 0.5061x_2 + 0.1041x_3 - 0.0109) + 1.0125)\}
\end{aligned}
$$

$$
\begin{aligned}
H_1(x) &= x \\
H_2(x) &= x^2 - 1 \\
H_3(x) &= x^3 - 3x
\end{aligned}
$$

A learning-based approach for uncertainty analysis

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Data Assimilation

Data assimilation fuses information from prior, model, and observations to reduce uncertainty.

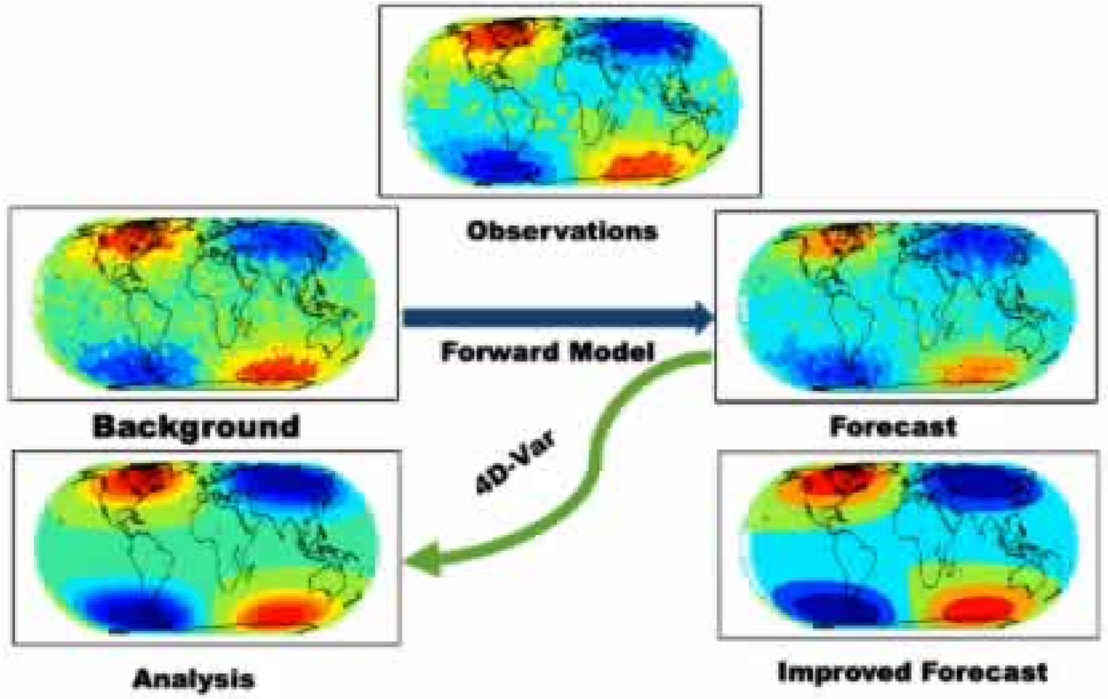
- We need to estimate the true state of the system($\mathbf{x}^{\text{true}}$)
- DA combines the following sources of information
  - **Prior** $\mathcal{P}^{\text{b}}(\mathbf{x})$: captures our current knowledge of $\mathbf{x}^{\text{true}}$
  - **The model**: captures our knowledge of the physical laws that govern the reality

$$\mathbf{x}_{k+1} = \mathcal{M}\left(\mathbf{x}_k\right) + \varepsilon^{\text{model}}, \quad k = 0, \ldots, N-1\,.$$

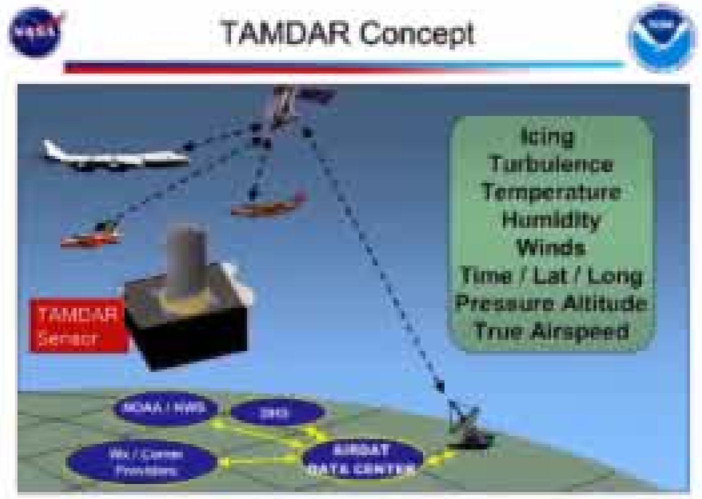
  - **Observations**: Noisy and sparse measurements of reality at different times

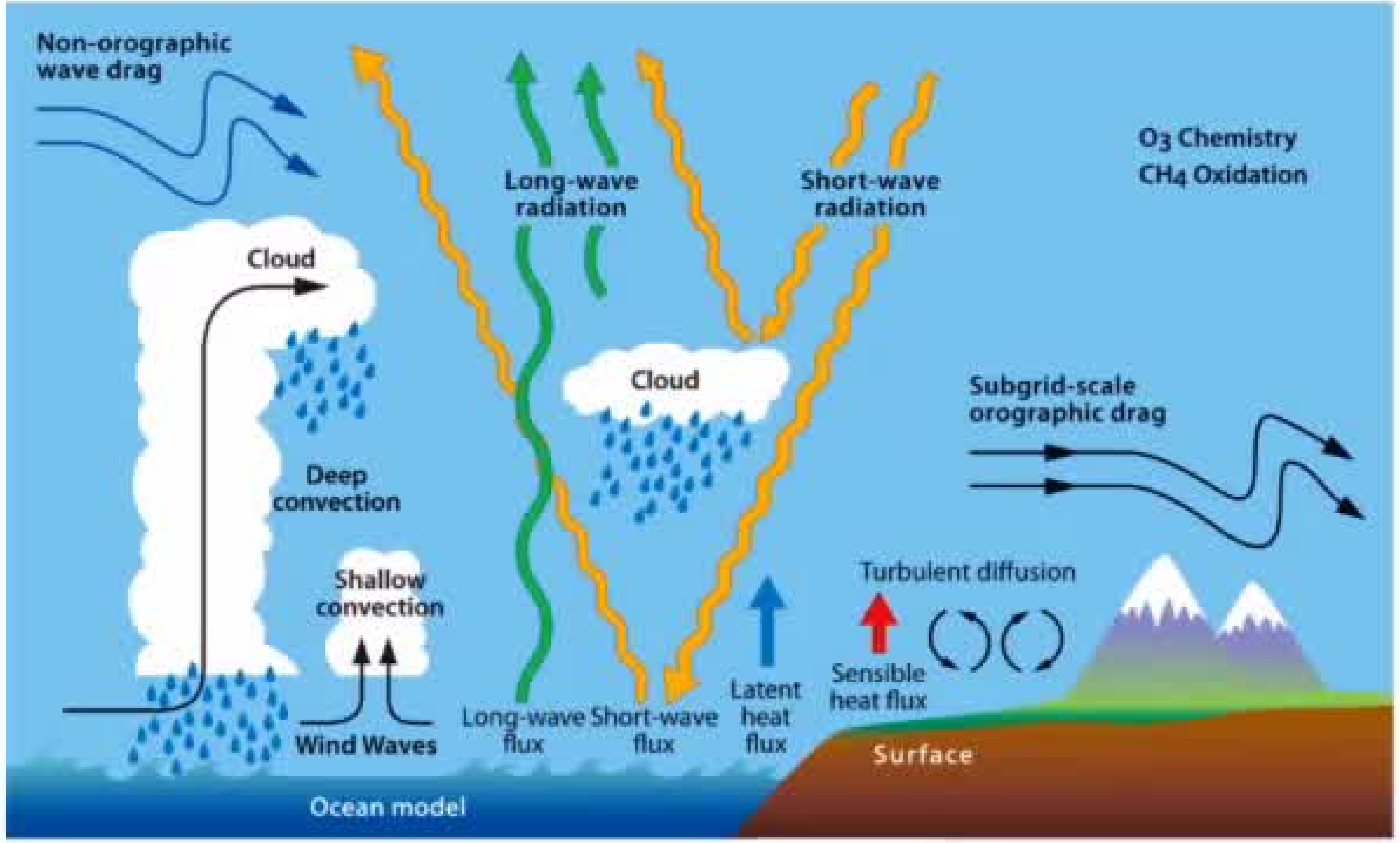
$$\mathbf{y}_i = \mathcal{H}_i\left(\mathbf{x}_i\right) + \varepsilon_i^{\text{obs}}, \quad i = 1, \ldots, N\,.$$

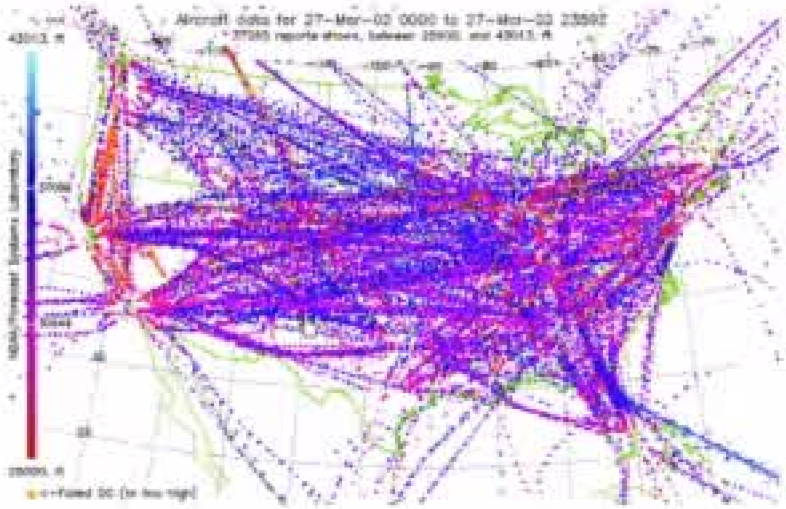
- DA computes the analysis (posterior, $\mathcal{P}^{\text{a}}(\mathbf{x})$) that represents our improved understanding of $\mathbf{x}^{\text{true}}$

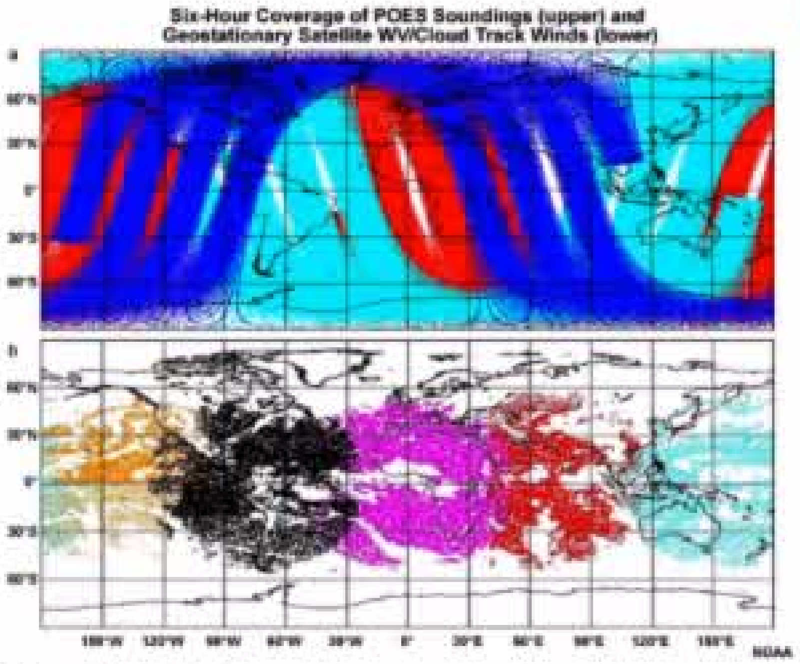


Challenges: Complex models and big data









- Complex Models (**10s of processes** and **10^8 Variables** in the state space).
- Lots and lots of data: **10^7** Observations from different sources in a period of 24 Hours.

Image sources: NASA, ECMWF, Weather.com

Model Errors

- We use measurements at sparse locations to obtain information about the global physical state

$$\mathbf{y}_t = h(v_t) + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \mathbf{R}_t), \quad t = 1, \cdots, T.$$

- The model predicted values at observed locations is given by

$$\mathbf{o}_t = \mathcal{H}(\mathbf{x}_t), \quad t = 1, \cdots, T.$$

- Hence the model error in observation space is:

$$\boldsymbol{\Delta}_t = \mathbf{o}_t - \mathbf{y}_t \in \mathbb{R}^m, \quad t = 1, \cdots, T.$$

- Hence we can write the evolution equations for the physical system:

$$\begin{aligned} v_t &= \mathcal{M}\big(v_{t-1}, \Theta\big) + \boldsymbol{\delta}_t(v_t), \quad t = 1, \cdots, T, \\ \mathbf{y}_t &= h(v_t) + \epsilon_t. \end{aligned}$$

Model Errors

- Consider the following NWP model that describes the time evolution of the atmosphere

$$\mathbf{x}_t = \mathcal{M}(\mathbf{x}_{t-1}, \Theta), \quad t = 1, \cdots, T\,.$$

- The atmosphere as an abstract process, evolves in time as follows:

$$v_t = \mathcal{P}\left(v_{t-1}\right), \quad t = 1, \cdots, T.$$

- The model state seeks to approximate the physical state:

$$\mathbf{x}_t \approx \psi(v_t), \quad t = 1, \cdots, T.$$

- Assuming that the model state at t – 1 has the ”ideal” value, the model prediction will differ from reality:

$$\psi(v_t) = \mathcal{M}\left(\psi(v_{t-1}), \Theta\right) + \boldsymbol{\delta}_t\left(v_t\right), \quad t = 1, \cdots, T.$$

Model Errors

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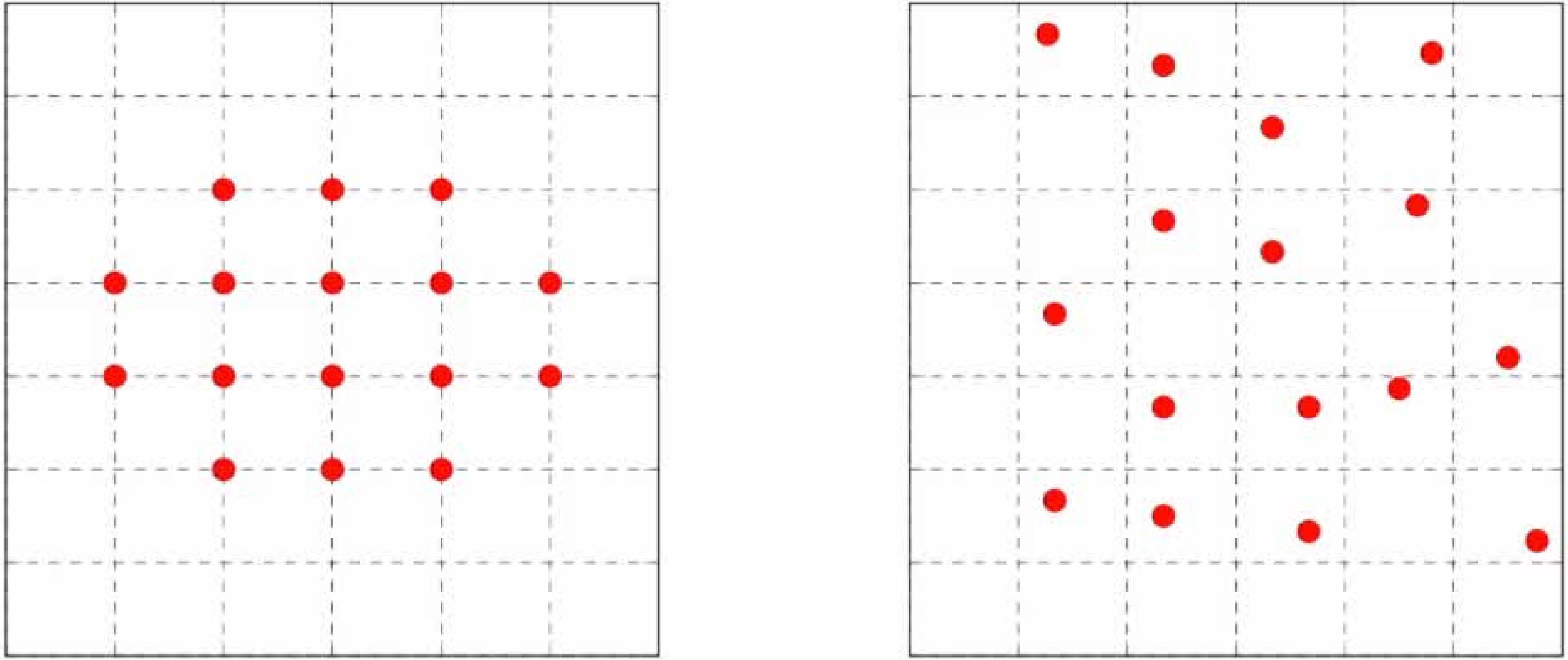
Observation operator ($\mathcal{H}$)



- Solution process involves some form of **comparison** between what the model predicts and the observations
- On the left: **Restrict** the solution to compare
- On the right: **Restrict + Interpolation** to compare

If we had access to the model errors

- Good estimates of the discrepancy when available, could improve model predictions by applying a correction:

$$\mathbf{v}_t \approx \mathbf{x}_t + \boldsymbol{\delta}_t.$$

- We are interested in the following problems

  - Estimating the QoI of the model error in advance

$$\phi^{\text{error}}\left(\Theta, \mathbf{o}_\tau, \boldsymbol{\Delta}_\tau, \mathbf{o}_t\right) \approx \boldsymbol{\Delta}_t \quad \tau < t.$$

  - Identifying the physical packages that contribute most to the forecast uncertainty

$$\phi^{\text{physics}}\left(\boldsymbol{\Delta}_t\right) \approx \Theta\,.$$

Numerical experiments

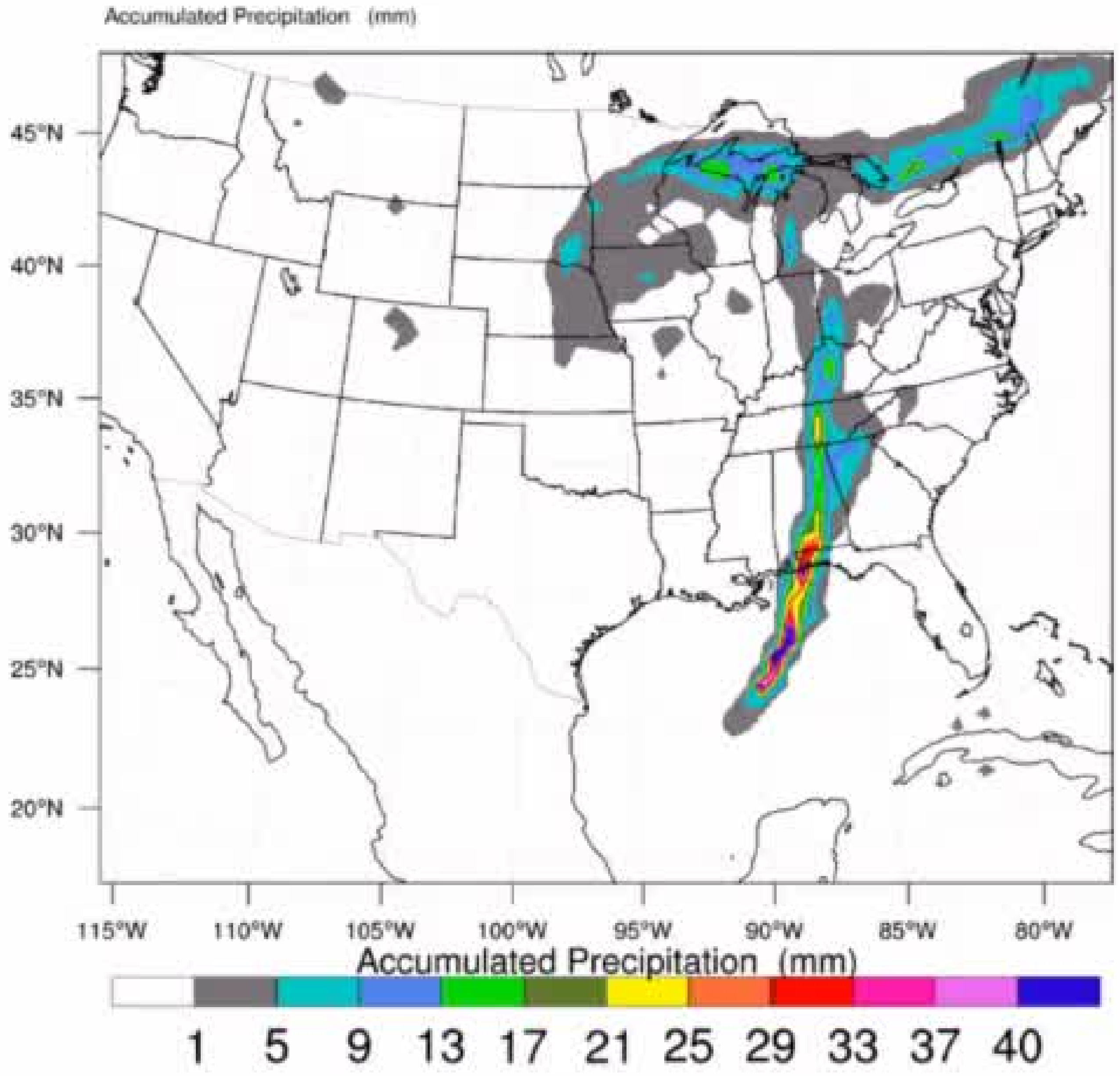
- All our experiments are conducted with WRF model and we estimate the uncertainties and model error for the prediction of precipitation.
- Training data: 7 AM to 12 AM (May 1st 2017).
- Testing period: 1 PM to 6PM (May 1st 2017).
- We use the "analysis provided" by NCEP as a proxy for truth.
- Input features which are used to train the machine

$$\phi^{\text{error}}\left(\Theta, \mathbf{o}_\tau, \boldsymbol{\Delta}_\tau, \mathbf{o}_{t=12\text{PM}}\right) \approx \boldsymbol{\Delta}_{t=12\text{PM}}, \quad 7\text{AM} \le \tau < 12\text{PM}.$$

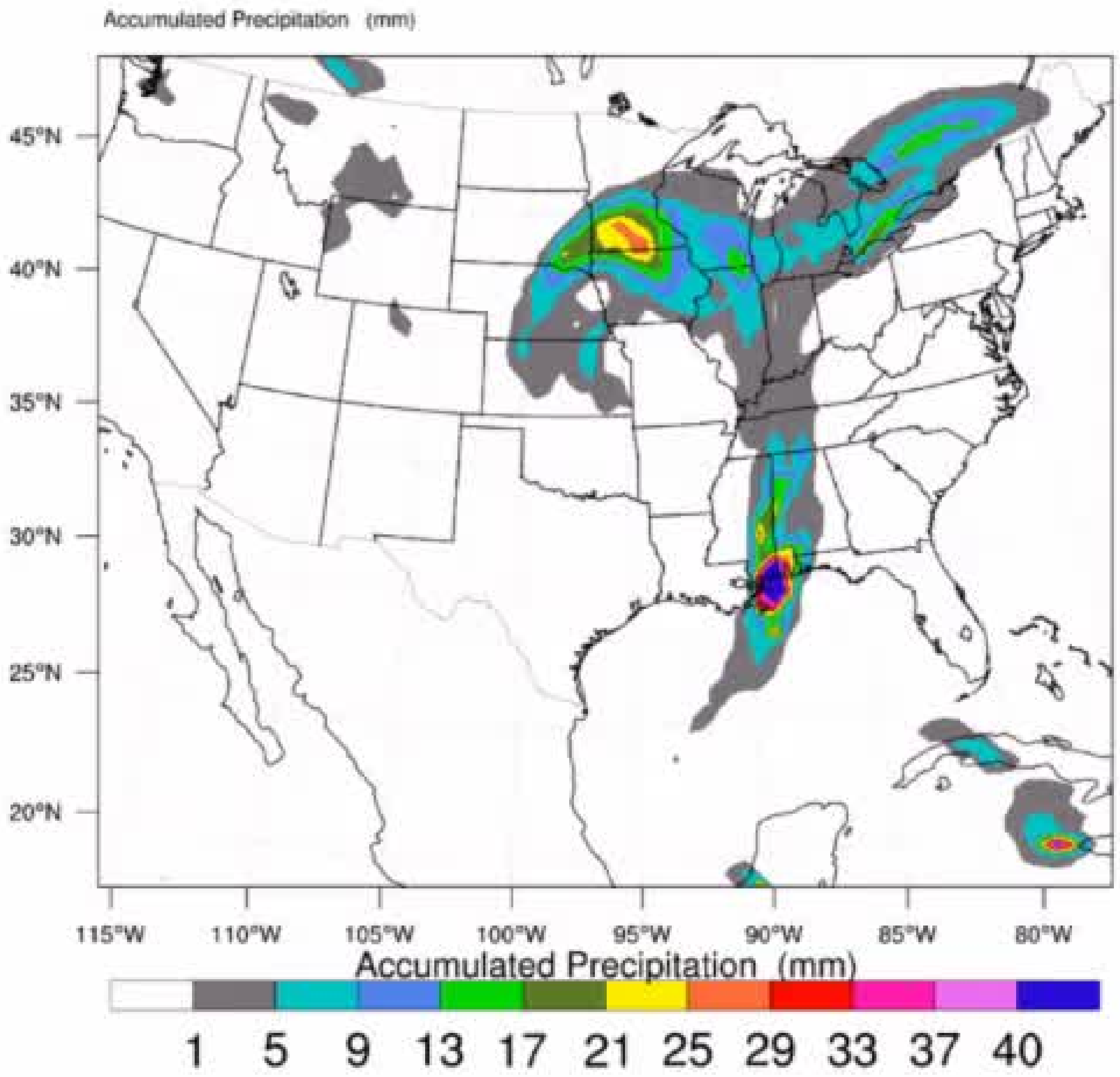
- Predict the forecast error at 6PM

$$\widehat{\boldsymbol{\Delta}}_{t=6\text{PM}} \approx \widehat{\phi}^{\text{error}}\left(\Theta, \mathbf{o}_\tau, \boldsymbol{\Delta}_\tau, \mathbf{o}_{t=6\text{PM}}\right), \quad 1\text{PM} \le \tau < 6\text{PM}.$$

Numerical experiments

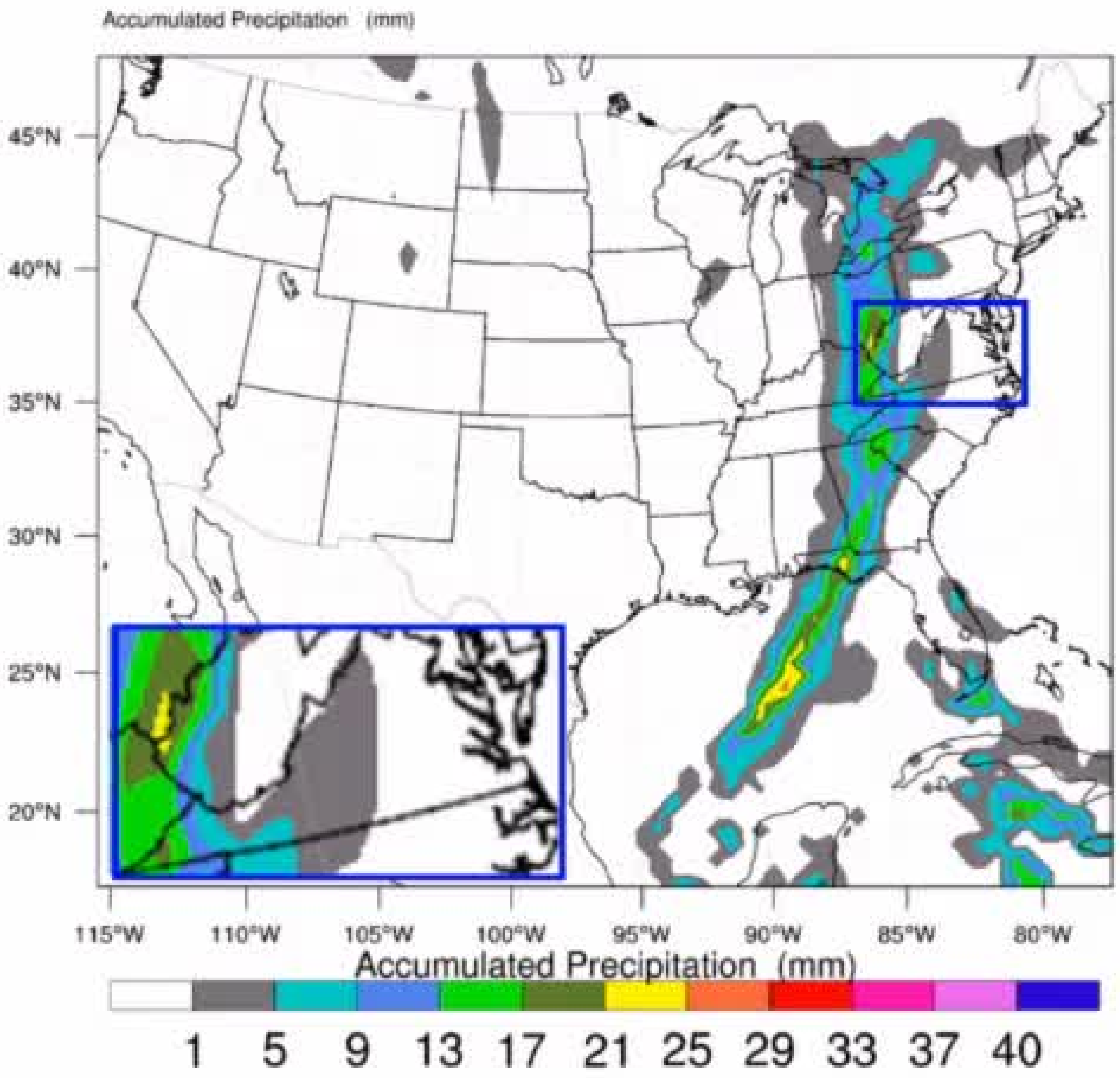


- Analysis at 6 AM
- Used as a proxy for truth for the training period

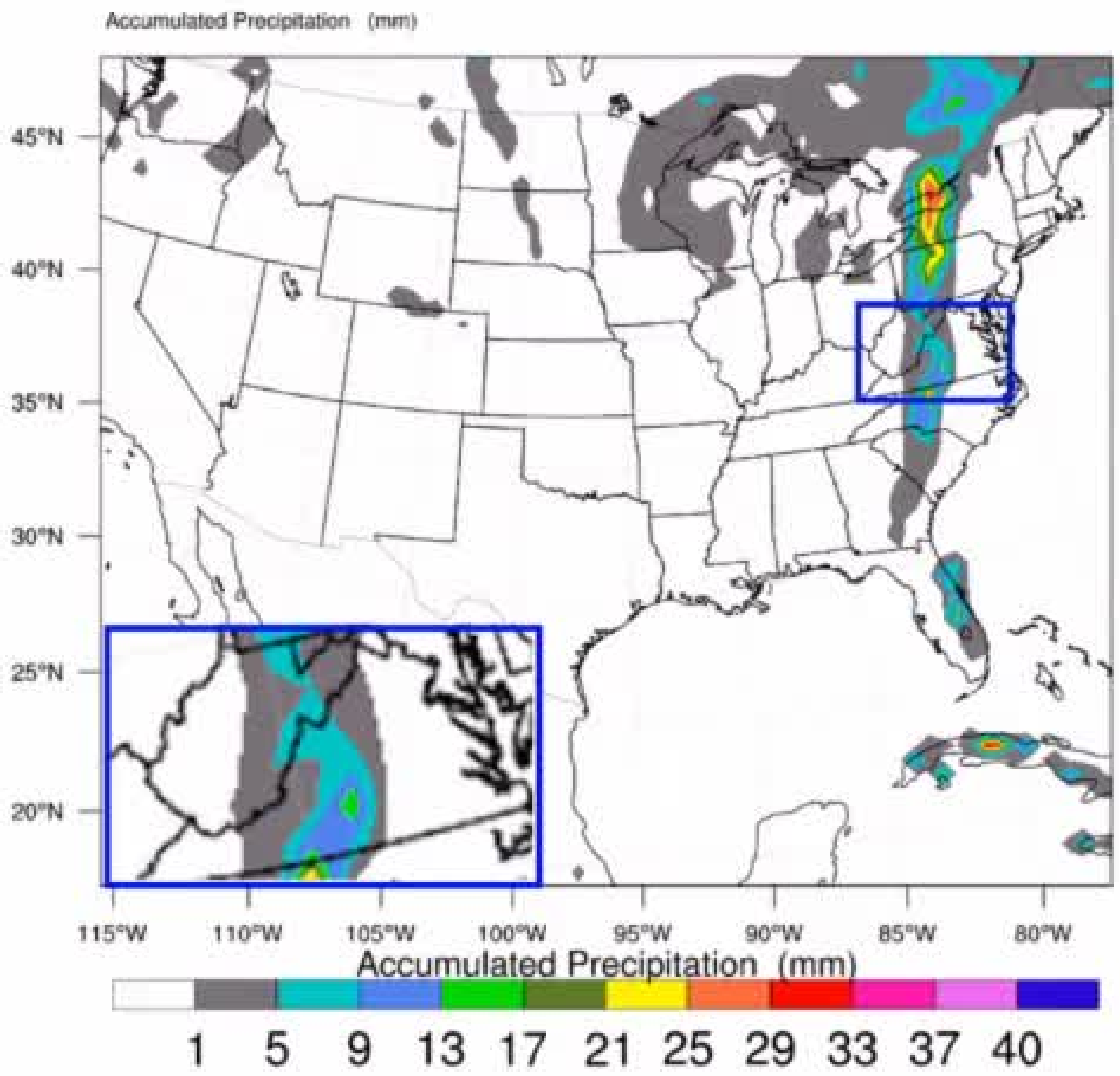


- Analysis at 12 PM
- Used as a proxy for truth for the testing period

Difference between WRF forecasts and Analysis

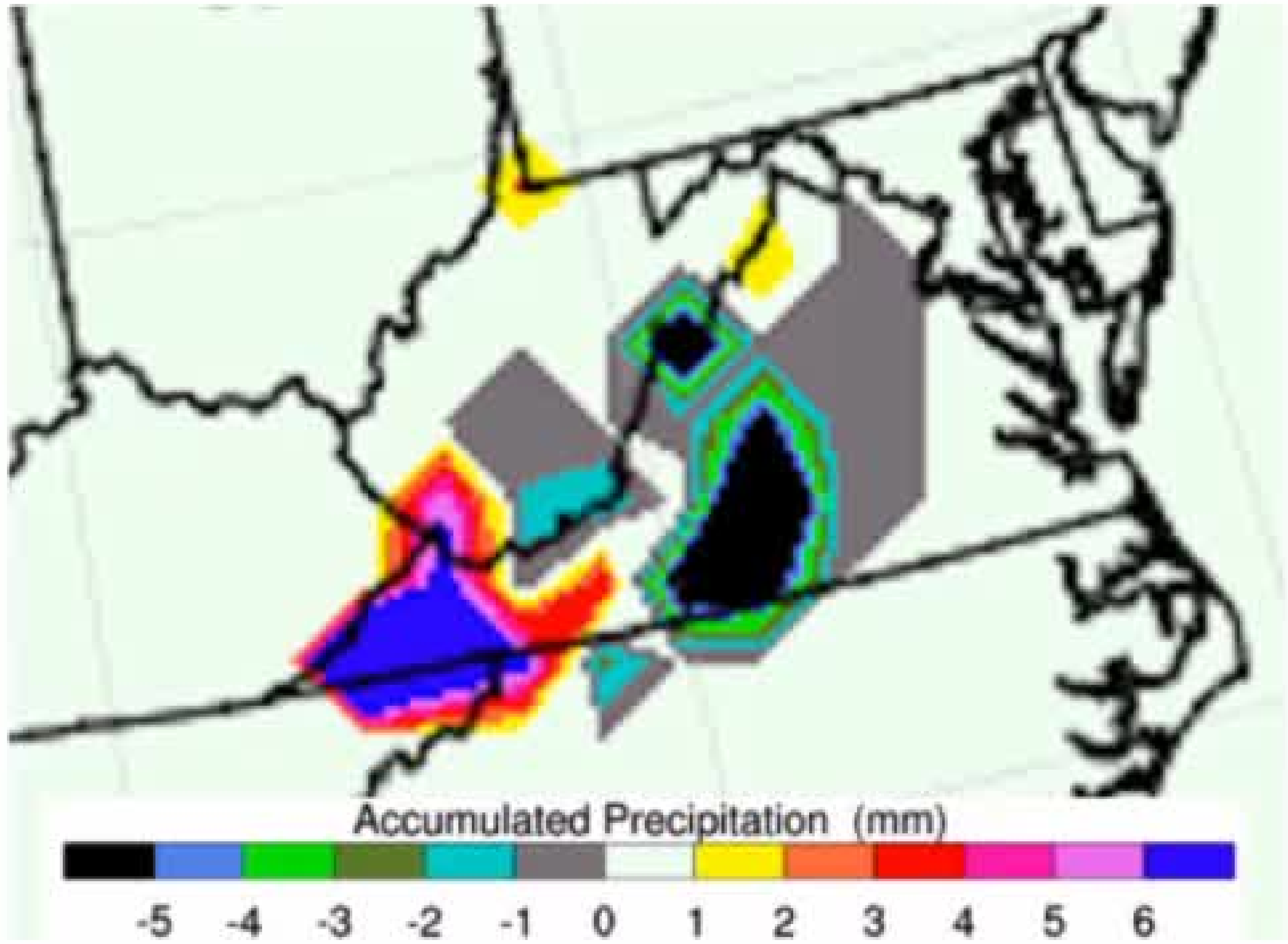


- WRF forecast at 6 PM



- NCEP Analysis at 6PM

Forecasts with and without corrections



- WRF Forecast
- WRF Forecast + Corrections

	RMSE
ANN	4.3 e-3
RF	5.8e-3

Packages that contribute to uncertainty

- The model configuration parameters represent various combinations of different physics such as microphysics schemes, cumulus parametrizations, short-wave, and long-wave radiation schemes
- The interaction of different physics schemes affect the accuracy of precipitation forecast.
- We construct a physics mapping using the norm and other statistical characterizations of the model data discrepancy as input features

$$\phi^{\text{physics}}\left(\bar{\mathbf{\Delta}}_{t=12\text{PM}}, \|\mathbf{\Delta}_{t=12\text{PM}}\|_2\right) \approx \Theta.$$

- WRF model is simulated for each of the possible physical combinations for the current forecast window and obtain the model errors for the current forecast window.
- From all the collected data, 80% is used for training the machine and on the remaining 20% we evaluate the model configuration, $\widehat{\Theta}_1$ for the given model errors.

Packages that contribute to uncertainty

- We repeat the test phase for each of the 50 samples with the scaled values of observable discrepancies ($\mathbf{\Delta}_{t=12\text{PM}}^{\text{test}}/2$) as inputs and obtain predicted physical combinations $\widehat{\Theta}_2$.
- The large variability in the predicted physical settings indicate that the WRF forecast error is sensitive to the corresponding physical packages.