Reduced Order Model for Global Atmospheric Simulation Data

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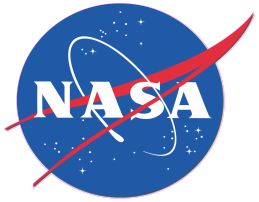
AMS 98th Annual Meeting
Monday, January 8, 2018



Goal

Global atmospheric chemistry data is simulated by a GEOS-Chem Chemical Transport Model (CTM) coupled with GEOS-5 Earth System Model (ESM)

Apply data-driven techniques to global atmospheric chemistry simulation data to build Reduced Order Models (ROMs) for the evolution of chemical species in the atmosphere

Analysis Methods

- Data Diagnostics

  Apply dimensionality reduction techniques *i.e.* compute the Empirical Orthogonal Functions (EOF) or Proper Orthogonal Decomposition (POD) to isolate leading-order features of chemical concentrations

- State reconstruction and Future State Prediction

  Apply Dynamic Mode Decomposition (DMD) that capitalizes the information from data diagnostics to build the ROMs

Data Diagnostics

1. Data slicing

   Slice the 3D-spatial grid (72 longitudes x 46 latitudes x 47 elevations) by fixing a latitude and elevation, traversing all 72 longitudes

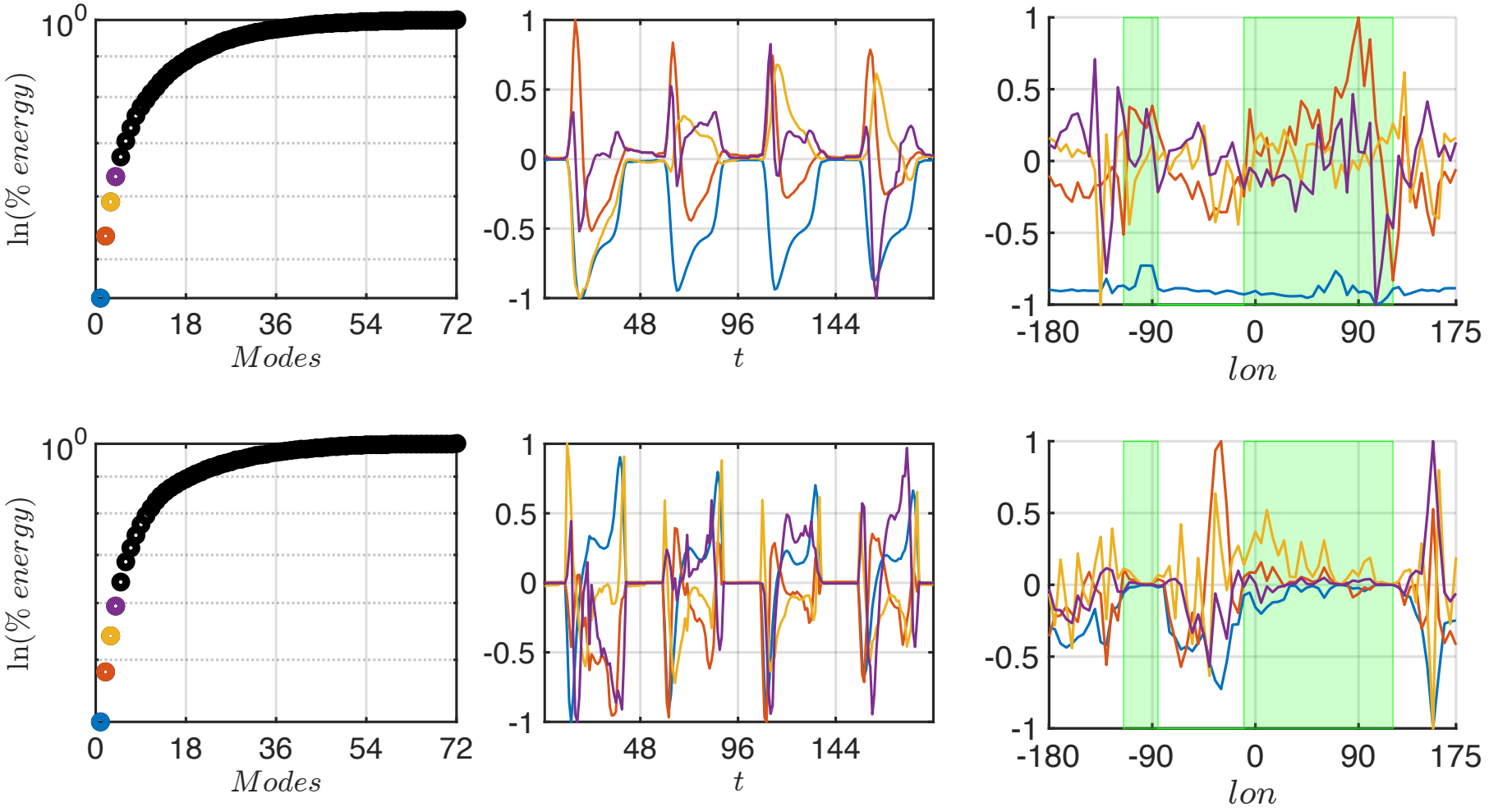
2. Data Preprocessing

   Normalize, Shift and Filter out any spurious spikes

3. Form the data matrix

   Stack the data from grid considered such that each column represents a different snapshot in time

POD/EOF Modes for NO at *lat*=30, *lev*=5

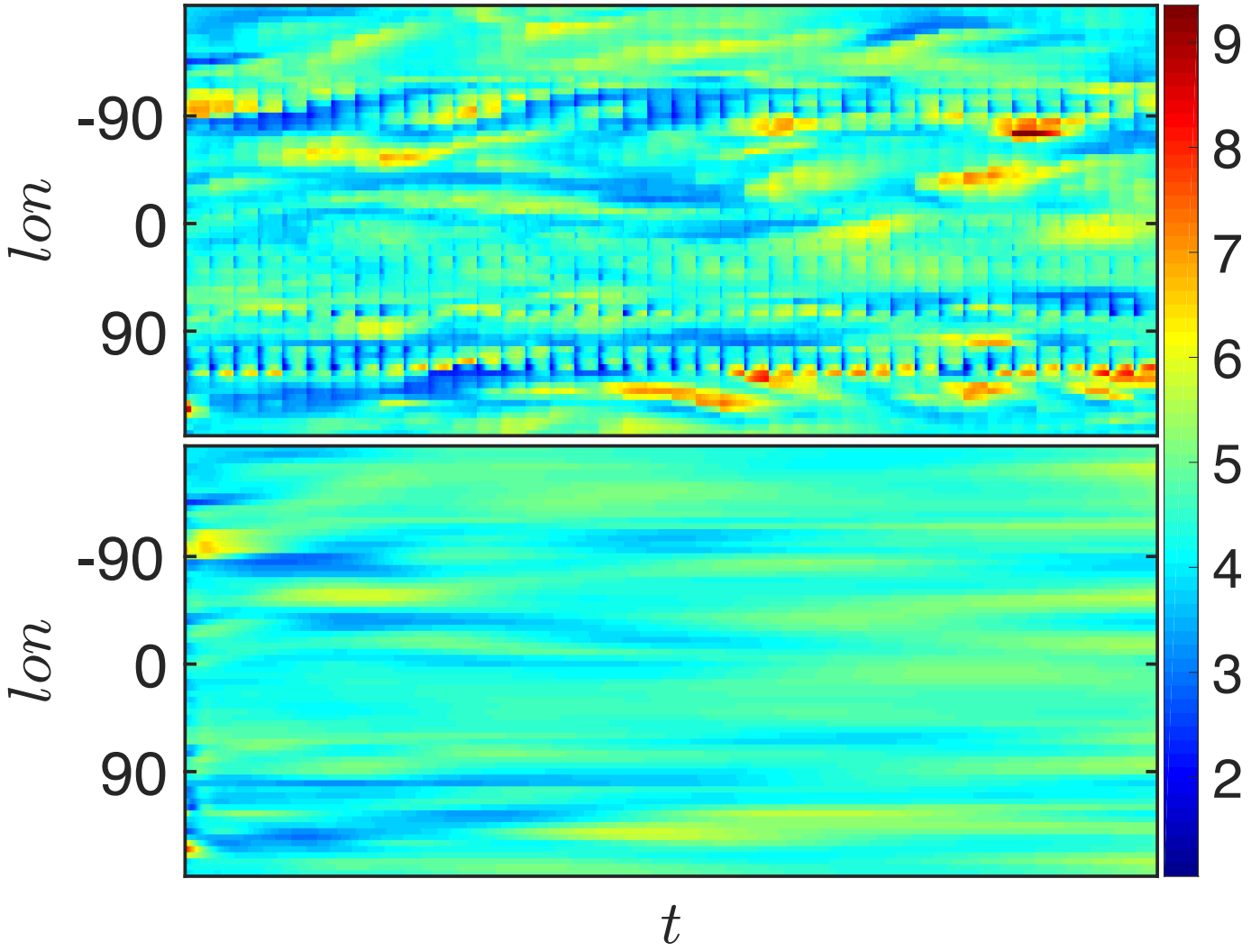


Dynamic Mode Decomposition

- The dynamic mode decomposition (DMD) is a leading tool for data driven modeling of dynamical systems, providing a regression framework for fitting linear dynamical models to time series measurement data
- Using the SVD of the snapshot matrix $\mathbf{X}$ the algorithm computes r DMD mode-eigenvalue pairs (φ_i, λ_i)
- Reconstruct and predict the system state by

$$\mathbf{x}(t) = \sum_{i=1}^{r} b_i \varphi_i e^{\log(\lambda_i) t/\Delta t}$$

Surface Ozone & classic DMD reconstruction at *lat*=30, for 40 days with 25 modes



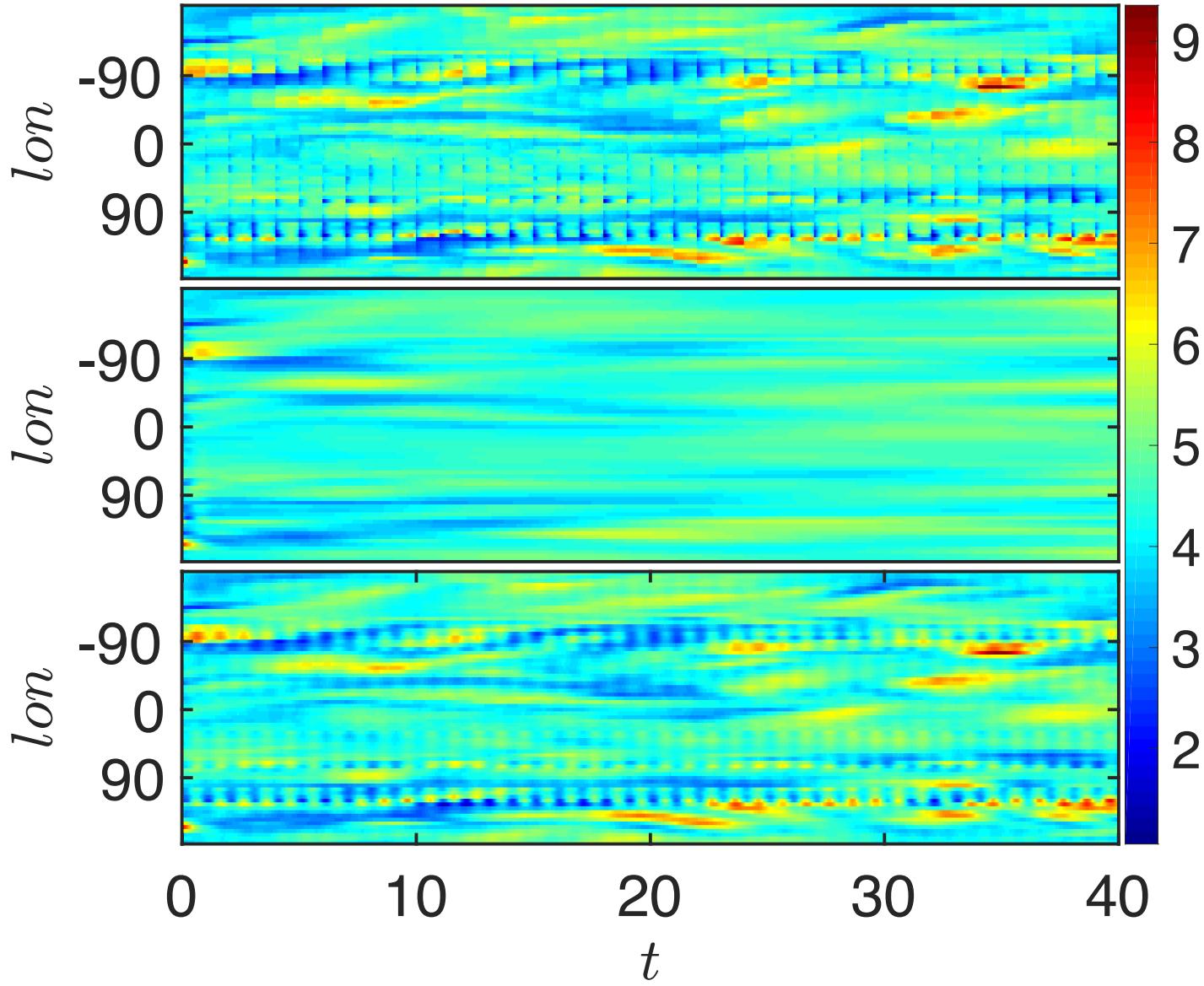
Explain optimized DMD

$$\mathbf{x}(t) = \sum_{i=1}^{r} b_i \varphi_i e^{\log(\lambda_i)t/\Delta t}$$

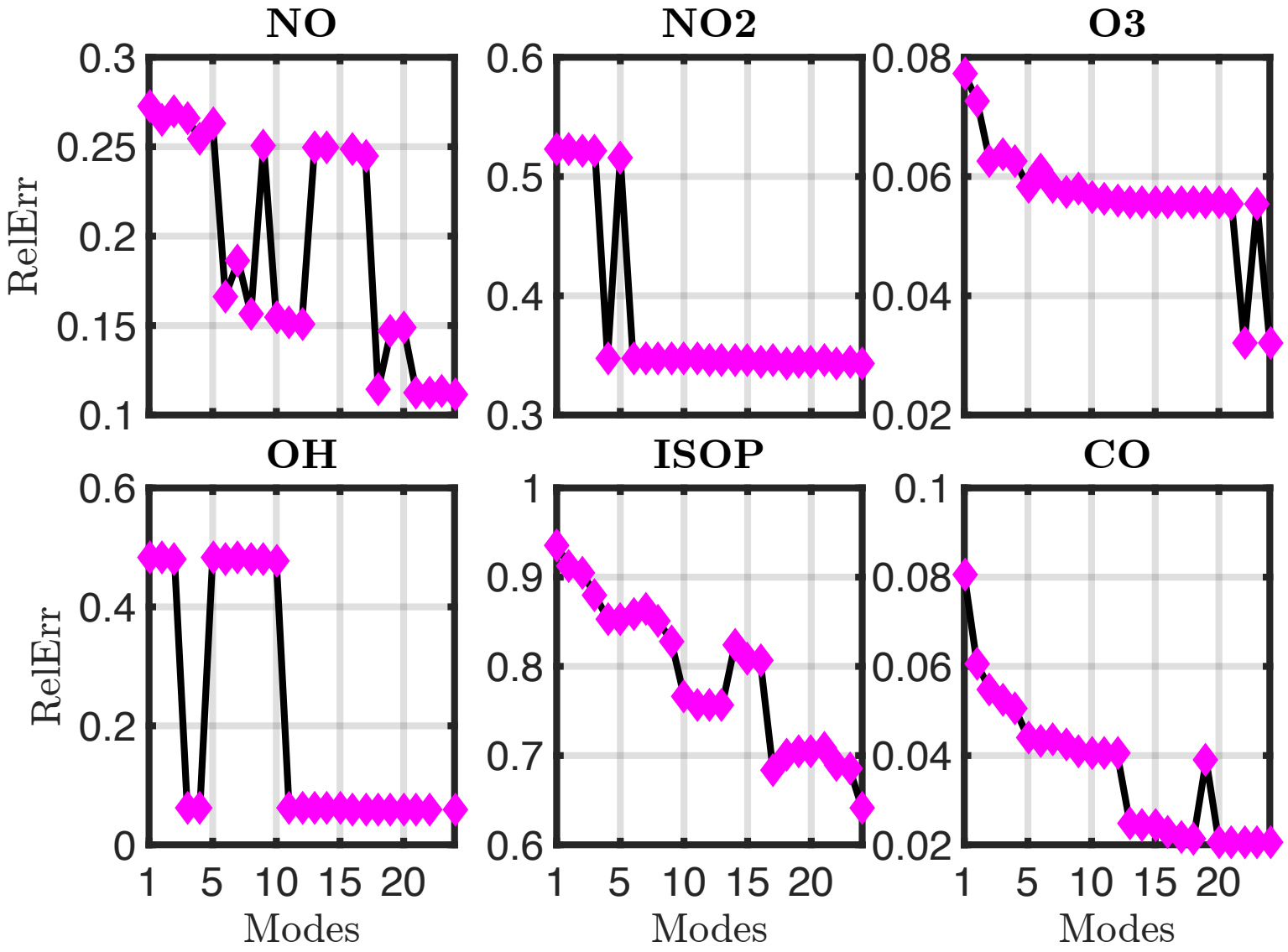
The Optimized DMD (OPTDMD) computes de-biased mode-eigenvalue-amplitude triad (ψ_i, λ_i, b_i) by solving the exponential fitting problem:

$$\text{minimize} \left\| \mathbf{X} - \begin{pmatrix} | & | & \\ \boldsymbol{\varphi}_1 & \boldsymbol{\varphi}_2 & \cdots \\ | & | & \end{pmatrix} \text{diag}(\mathbf{b}) \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^m \\ 1 & \lambda_2 & \cdots & \lambda_2^m \\ \vdots & \vdots & \ddots & \vdots \end{pmatrix} \right\|_F$$

Surface Ozone, classic DMD and OPTDMD reconstruction at *lat*=30, for 40 days with 25 modes

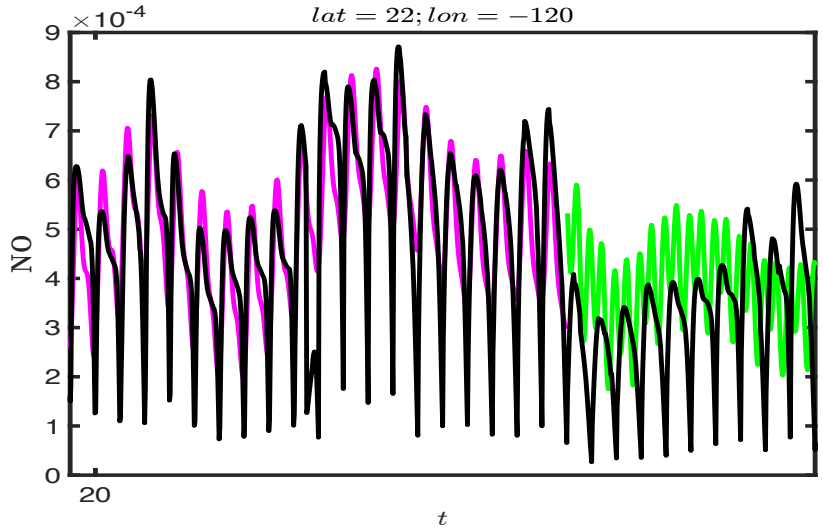


Relative errors for OPTDMD reconstruction



Summary

- Our data-driven diagnostics show a consistent pattern of low dimensional features across the global chemistry landscape, thus demonstrating that ROM architectures are capable of reconstructing low-rank models.
- OPTDMD reconstructs the chemical concentration time series using only the leading-order modes
- Current research: Future state estimation



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