Accelerated MCMC for OCO-2's CO_2 Retrieval

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Finnish Centre of Excellence in Inverse Modelling and Imaging 2018-2025

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NASA JPL Jet Propulsion Laboratory California Institute of Technology

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Finnish Centre of Excellence in Inverse Modelling and Imaging 2018 – 2025

A research project to combine important application areas and world leading mathematics in inverse problems and uncertainty quantification.

FMI's interest:
remote sensing,
climate and weather,
carbon cycle,
air quality, ozone

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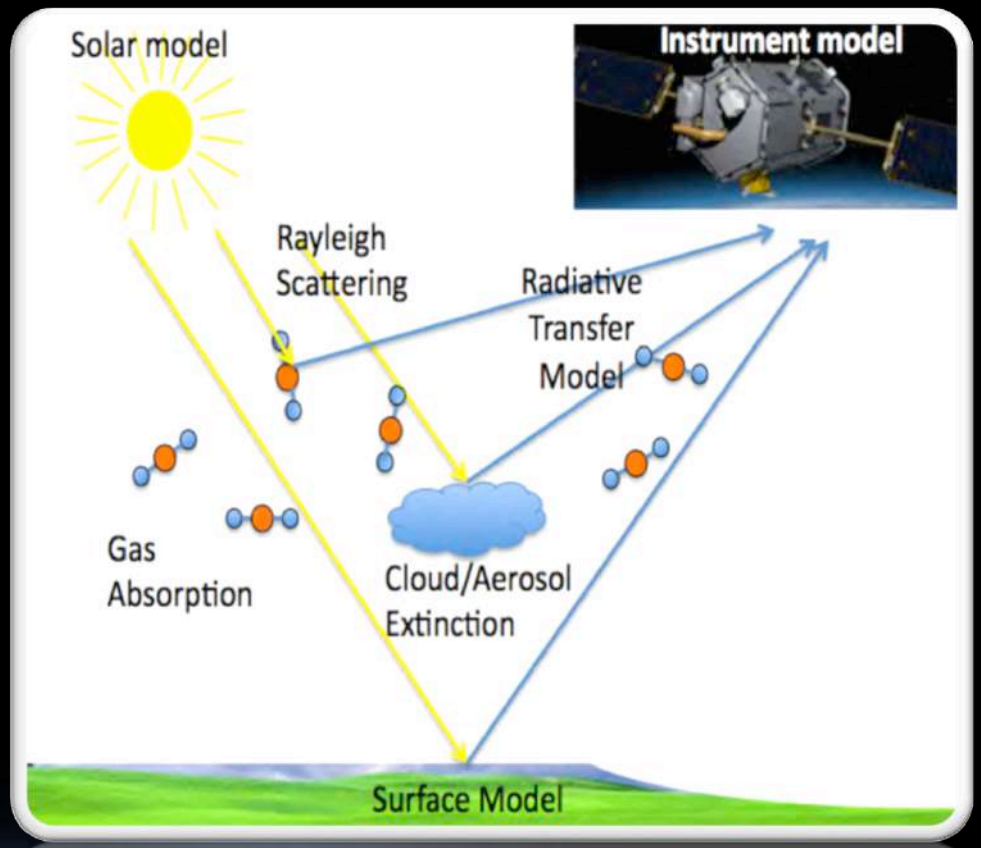
Outline

- OCO-2 surrogate model
- Inverse Problem
- MCMC & Dimension Reduction
- Results

Orbiting Carbon Observatory 2

Picture: NASA, JPL



Full Physics Model, Picture: NASA JPL

Carbon dioxide monitoring mission by NASA Jet Propulsion Laboratory, launched on and operational since July 2014.

Problem Setup

Surrogate model state vector [Hobbs et al. 2017]

$x_1 – x_{20}$ - CO_2 profile

x_{21} - Surface pressure

$x_{22} – x_{27}$ - Surface albedo

$x_{28} – x_{39}$ - Aerosols

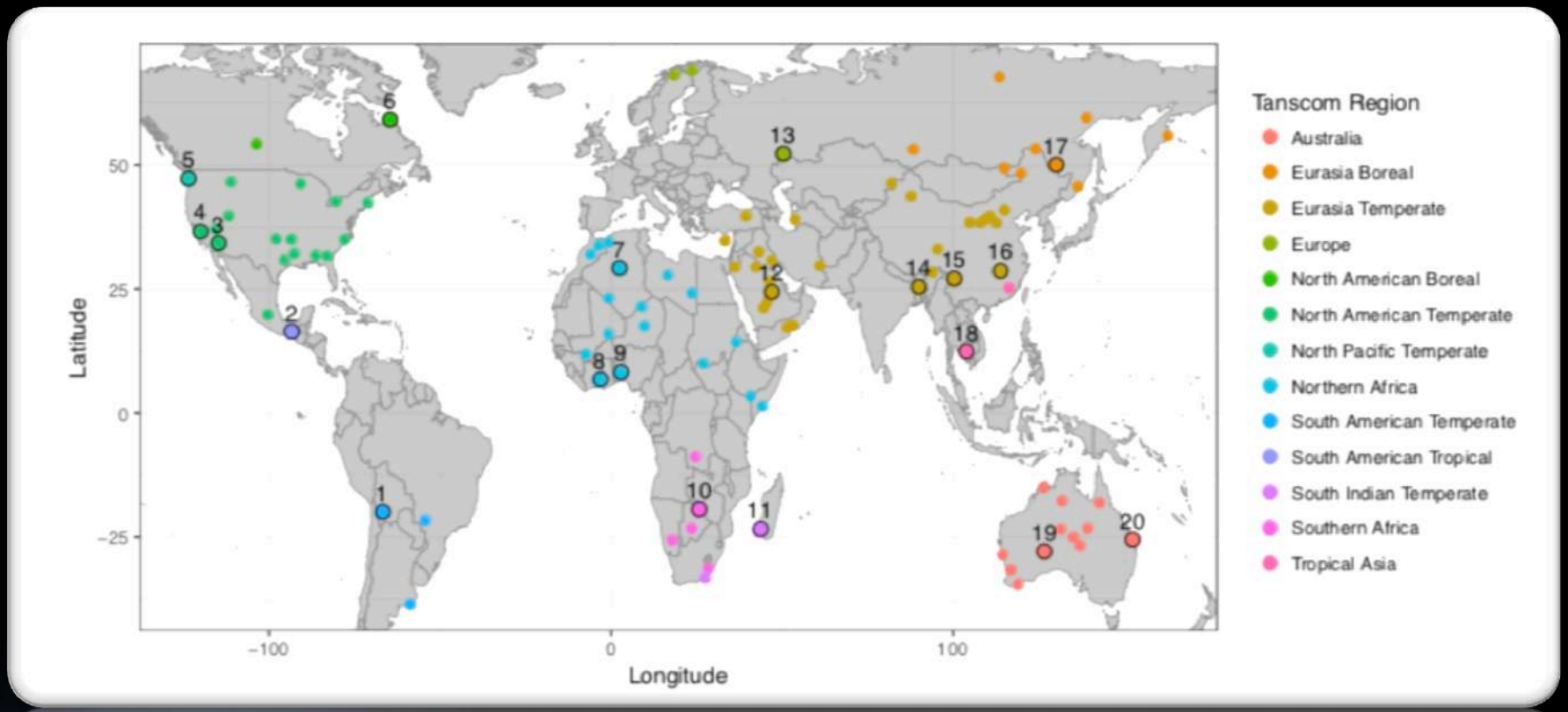
Component	Full Physics	Surrogate
20-Level CO_2 profile	✓	✓
Surface air pressure	✓	✓
Surface albedo	✓	✓
Aerosol profile	✓	✓
Temperature scaling	✓	
Humidity scaling	✓	
Wavelength offset, scaling	✓	
Fluorescence	✓	

Problem Setup

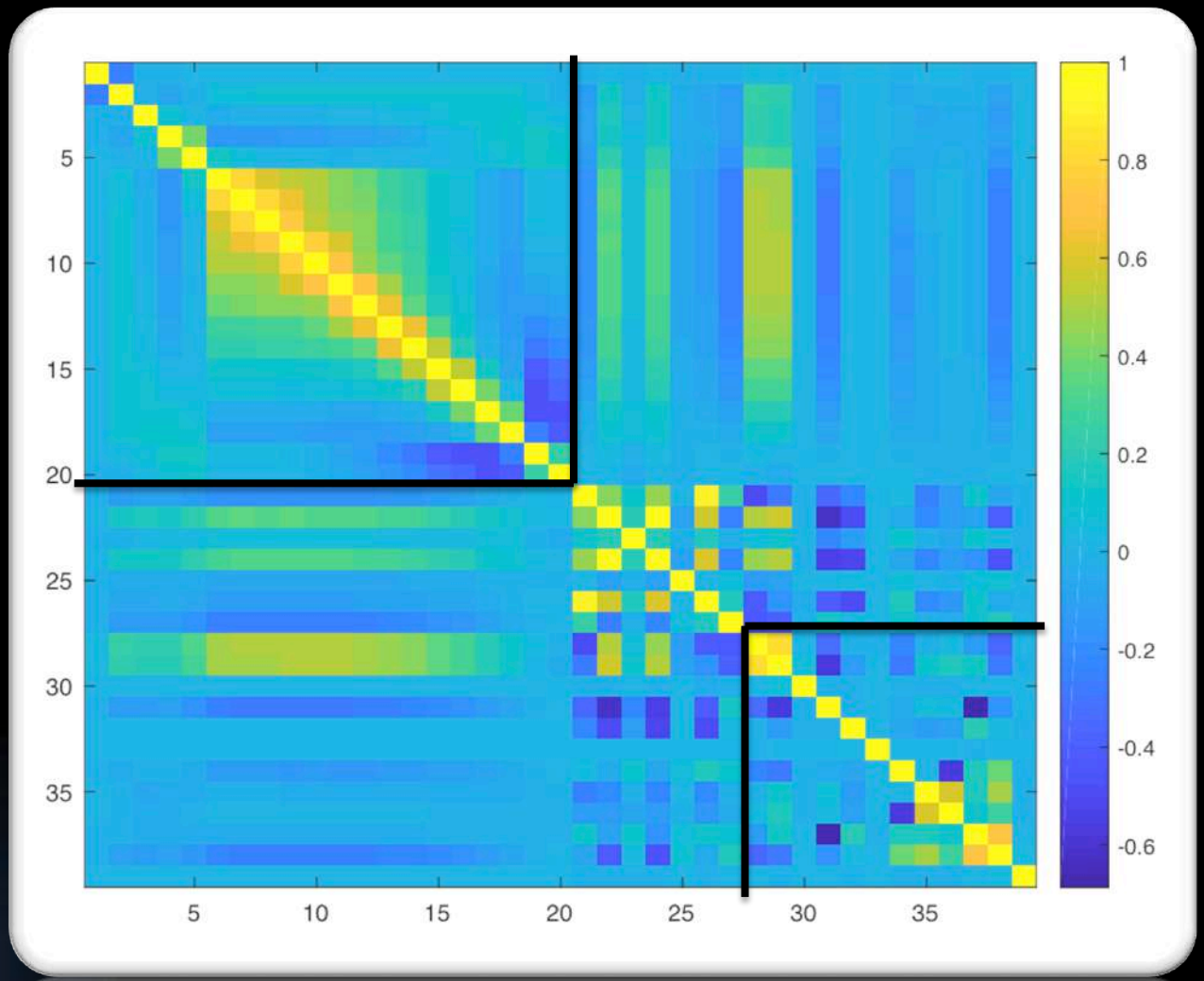
Simulated state vectors [Brynjarsdottir et al 2018] drawn from a normal distribution with empirical mean and covariance given by:

- Vertical CO_2 profiles: NASA's Goddard Earth Observing System Model, version 5 (GEOS-5).
- Surface pressure and aerosols: Modern Era Retrospective Analysis for Research and Applications Aerosol Reanalysis (MERRAero).
- Surface albedo: Moderate Resolution Imaging Spectrometer (MODIS) albedo product

MCMC test case: tmp001



Posterior Correlation Matrix



Problem Setup

Inverse Problem:

$$y = F(x) + \varepsilon, \qquad x_{pr} \sim N(x_0, \Gamma_{pr}), \varepsilon \sim N(0, \Gamma_\varepsilon)$$

Bayesian Solution: Posterior distribution

$$\pi(x|y) \propto \pi_\varepsilon(y|x)\pi_{pr}(x)$$

Optimal estimation: $N(x_{\mathrm{MAP}}, \widehat{S})$

$$x_{\mathrm{MAP}} = \mathrm{argmin}_{\mathrm{x}} - 2\ln\left(\pi(\mathrm{x}|\mathrm{y})\right)$$

$$\widehat{S} = \left(J(x_{\mathrm{MAP}})^T \Gamma_\varepsilon^{-1} J(x_{\mathrm{MAP}}) + \Gamma_{pr}^{-1}\right)^{-1}$$

Problem Setup

Markov Chain Monte Carlo (MCMC):

$$\text{Propose } x_t \sim N(x_{t-1}, C), \text{accept/reject with } \min\left(\frac{\pi(x_t|y)}{\pi(x_{t-1}|y)}, 1\right)$$

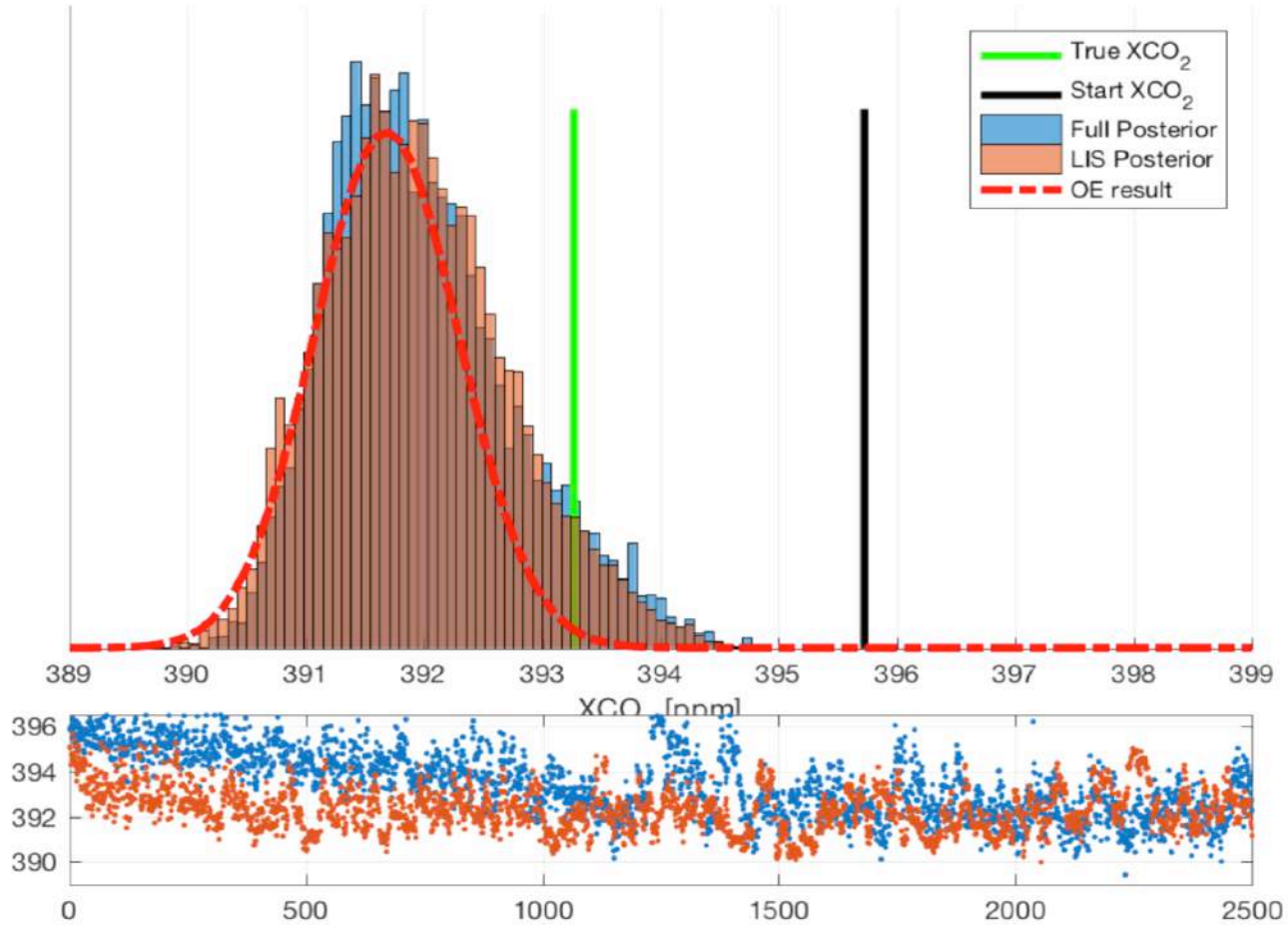
Adaptive MCMC:

$$C_t = \begin{cases} C_0, & t < t_0 \\ s_d \mathrm{cov}\left[X_0, \ldots, X_{t-1}\right] + s_d \varepsilon I, & t \geq t_0 \end{cases}$$

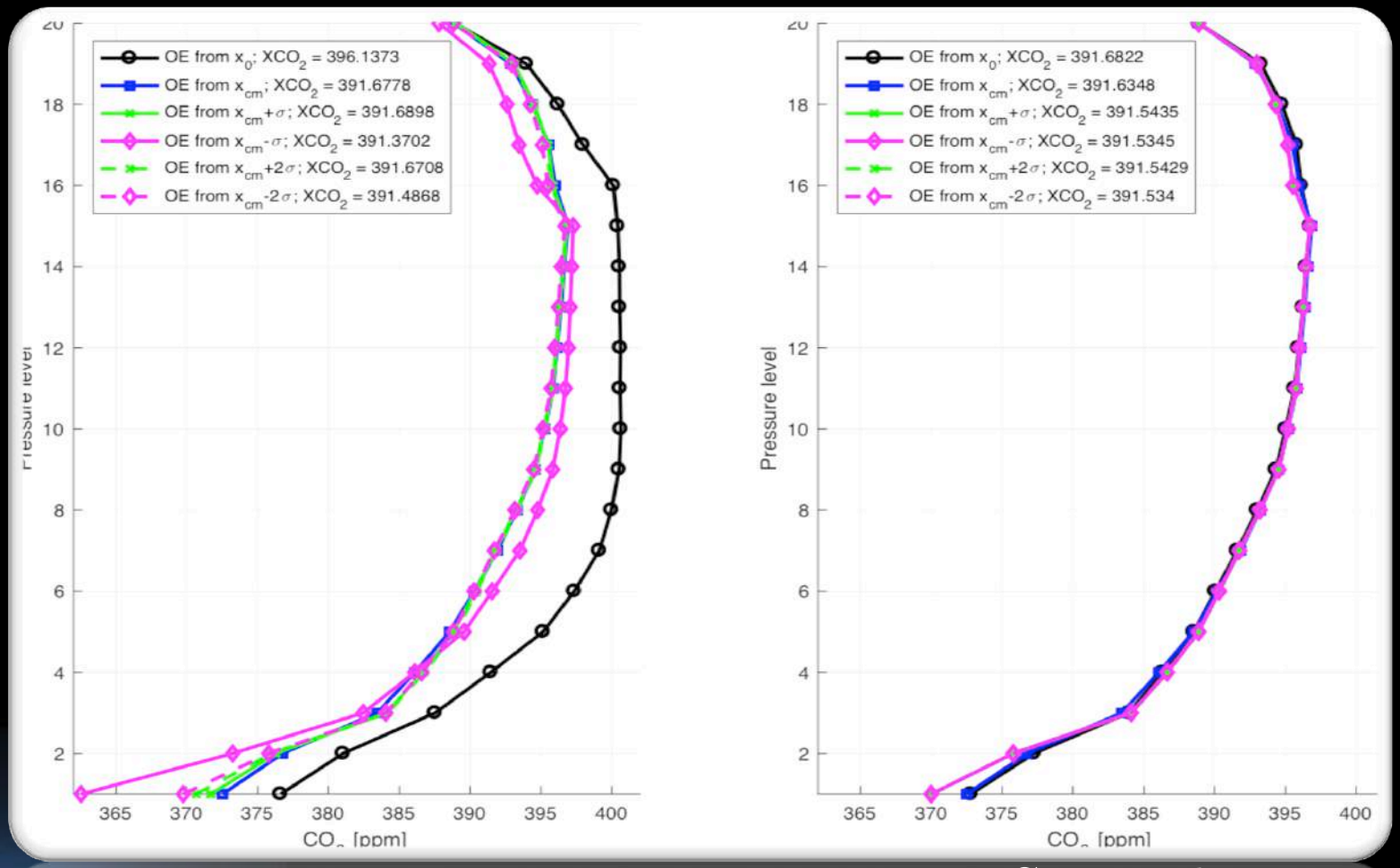
Dimension reduction:

$$x = P_r x_r + P_\perp x_\perp, \quad \pi_r(x_r|y) \propto \pi_\varepsilon(y|x_r)\pi_{pr}(x_r)$$

XCO_2 from MCMC

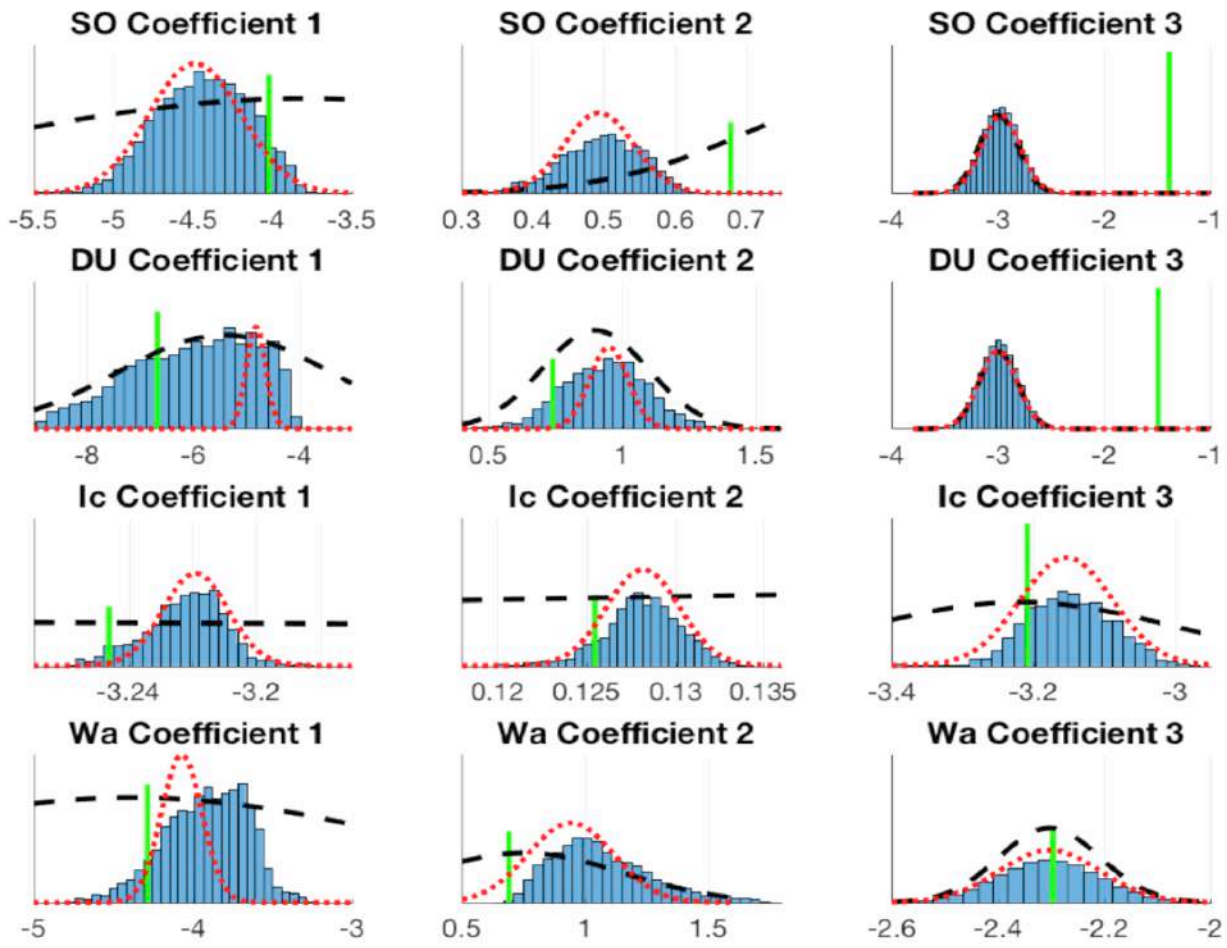


Optimal Estimation w/ different first guess

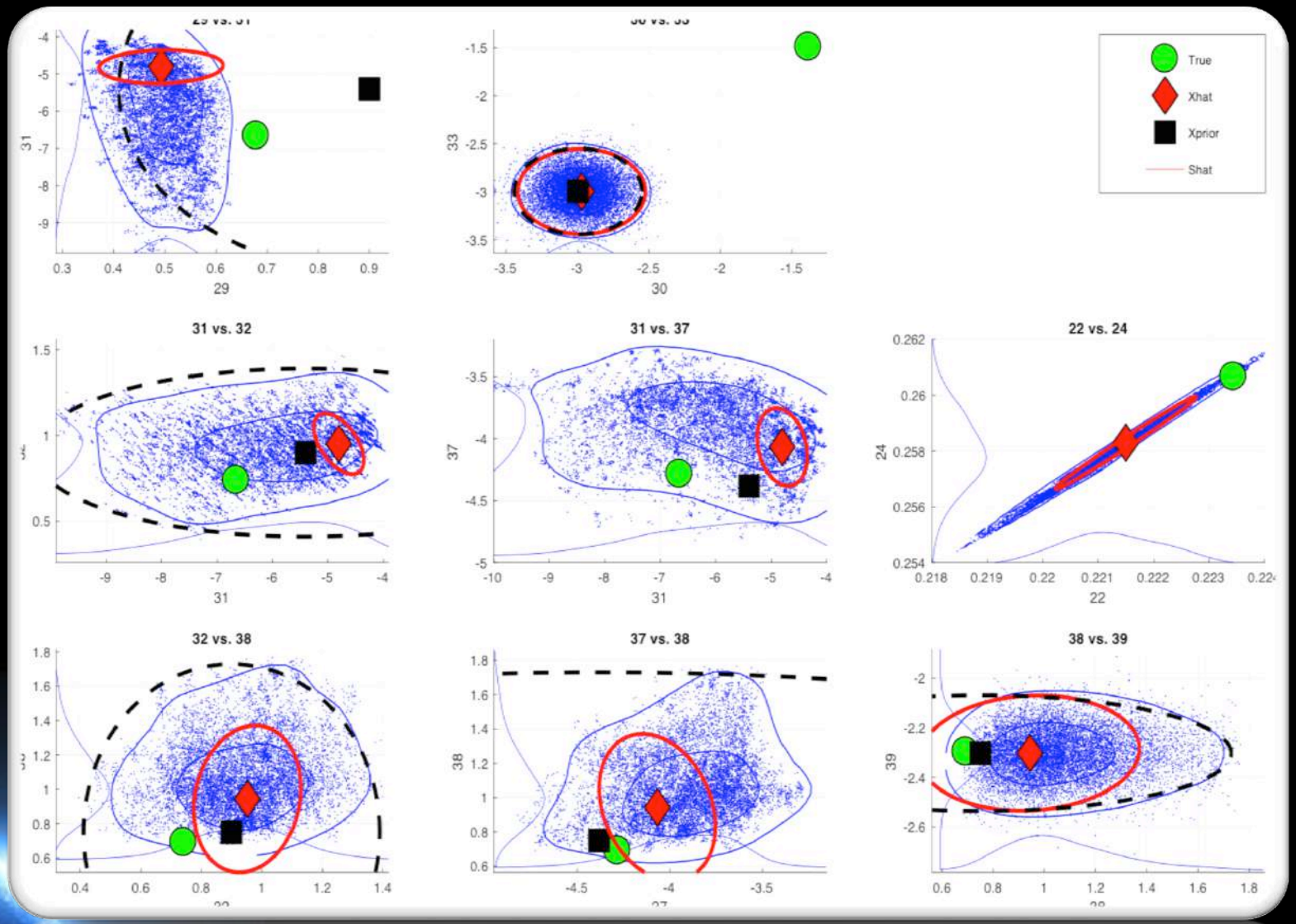


$\gamma = 10, \quad \text{Step tol.} \ = 40 \qquad \gamma = 30, \quad \text{Step tol.} \ = 10^{-4}$

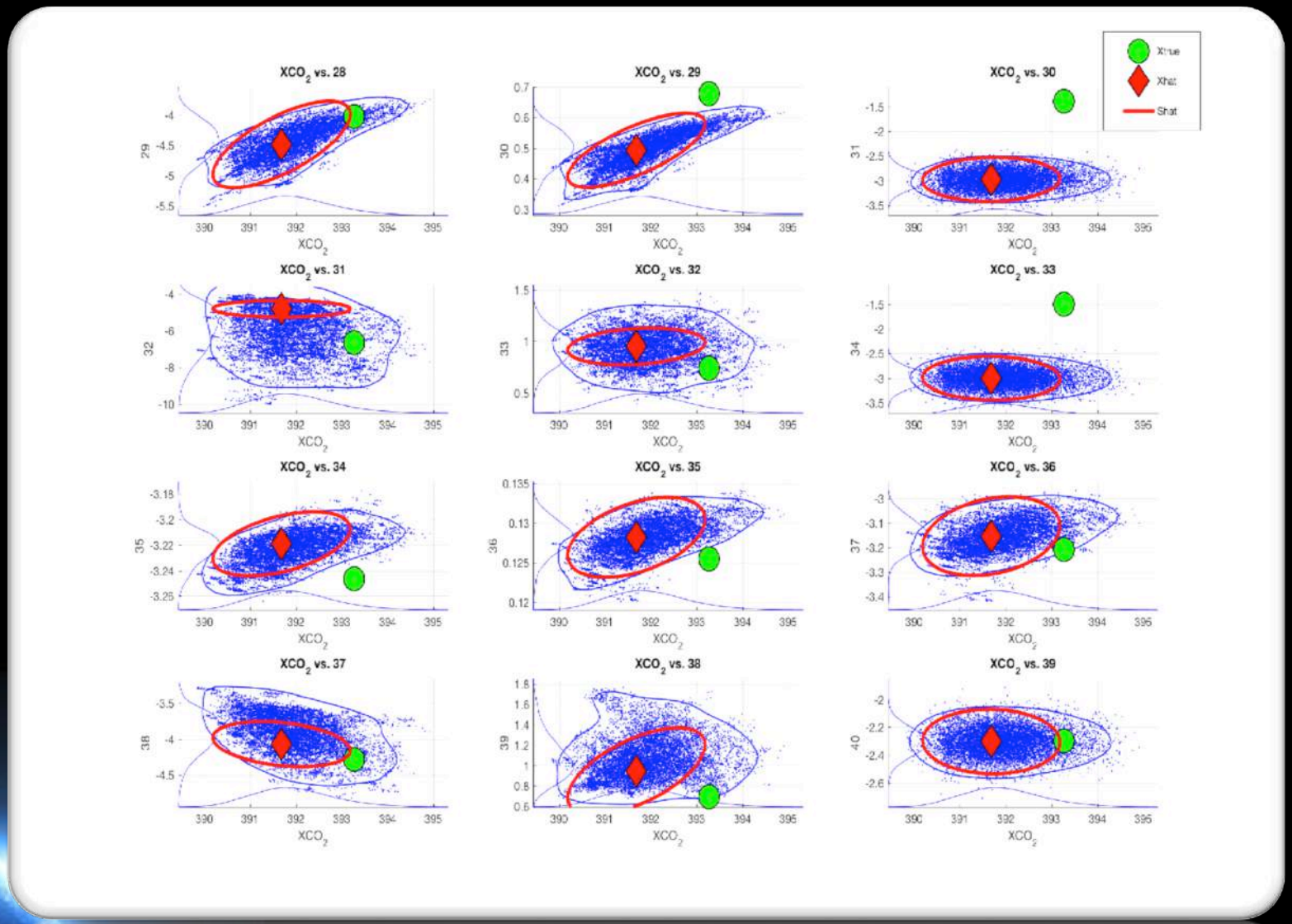
Posterior histograms for Aerosols



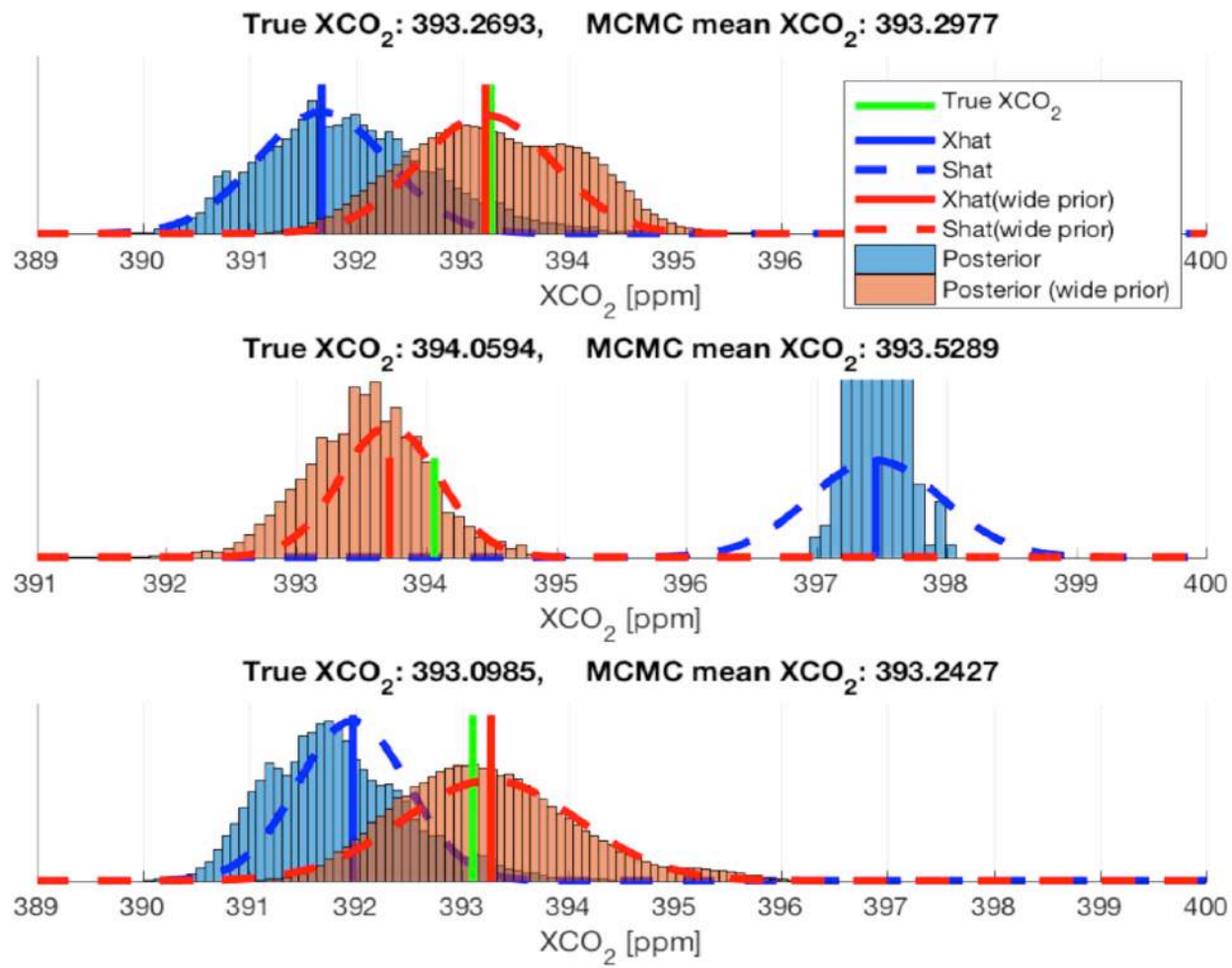
2D Posterior plots: aerosols



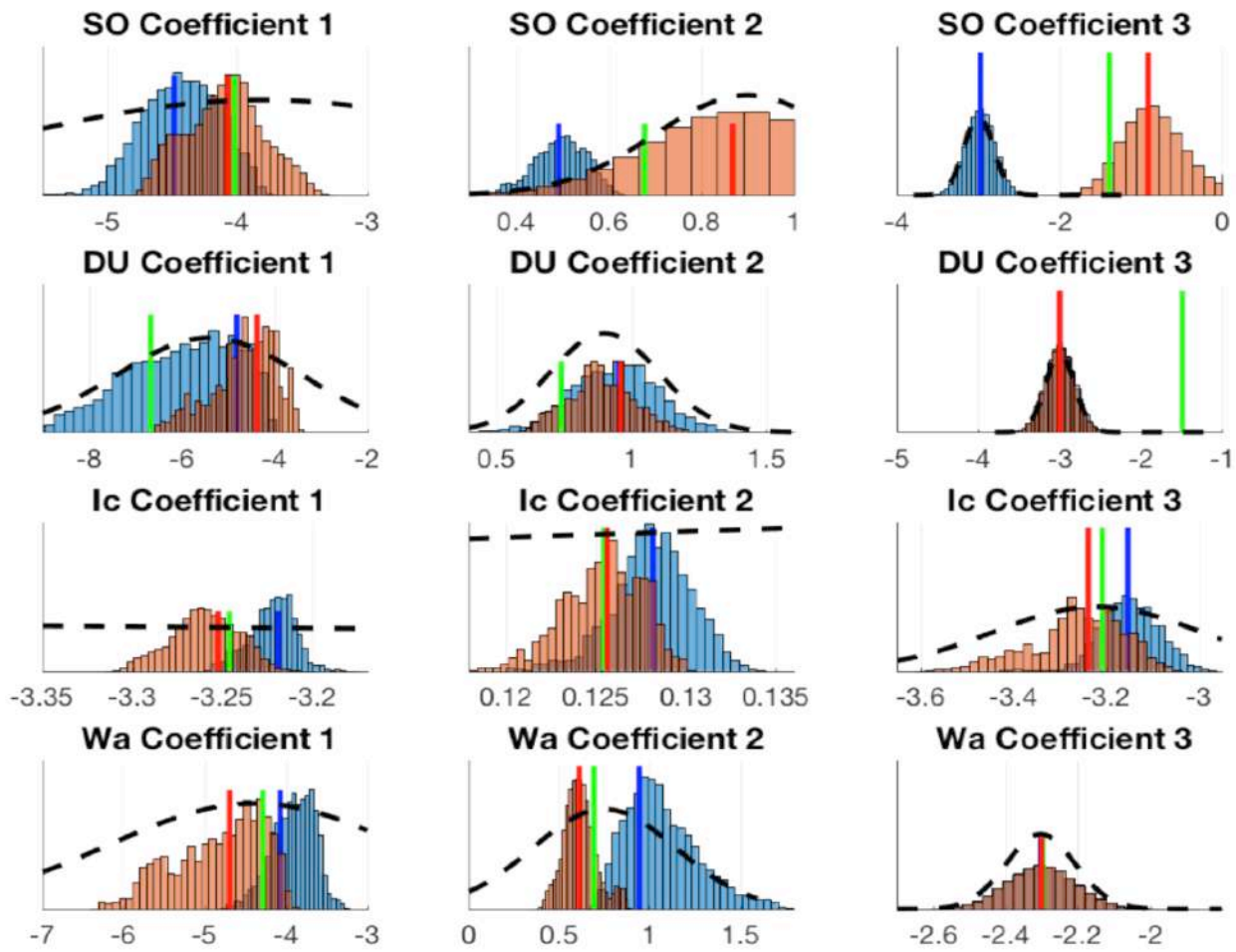
2D Posterior plots: XCO_2 vs. Aerosols



Posterior XCO_2 with looser prior



Posterior Aerosols with looser prior



Ongoing / future efforts

- Surrogate vs Full Physics
- Identification of problematic geolocations / aerosol types
- In-depth look at operational prior covariance matrix

References

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Thank you!

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